# Methoden der

# Hartree-Fock-Bogoliubov Theorie


vorgelegt von

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# Contents

# Introduction

The aim of the present work is to elaborate on an approximation method in quantum mechanics, known as Hartree-Fock-Bogoliubov-Theory (HFB-Theory) or as Generalized Hartree-Fock-Theory. A good introductory reading to this topic is [11], for a good account on fermionic HFB-Theory, see [8]. The object is to gain as much information as possible on the ground state energy (density) of a quantum mechanical system, defined to be the largest lower bound on all possible energy (density) expectation values. This quantity is in most cases inaccessible to direct computation, and thus the idea of HFB-Theory is to produce an upper bound of the ground state energy (density), by evaluating the infimum over a restricted set of states, namely the set of quasi-free states. This set of states is characterized by the property that all the correlation functions of such a state may be expressed entirely in terms of one-point and two-point correlation functions, by the so called Wick Theorem. This class of states is quite large, covering in particular all Gibbs states associated to quadratic Hamiltonians, and therefore one might hope that the upper bound is not too far away from the real ground state energy. However, in order to control the quality of this upper bound, or in particular to estimate the ground state energy (density) from below, it is necessary to provide estimates of the approximation error. This is achieved by correlation estimates.

We proceed as follows:

In Chapter 1 we give a summary of the theory of quantum many-particle systems, obeying fermion or boson statistics. Most of the proofs we present in that chapter are taken from [13]. The two fundamental objects in quantum many-particle theory we introduce are the CAR and CCR Algebras, generated by operator-valued functionals

$$f \mapsto a^*(f) \qquad \text{and} \qquad f \mapsto a(f) \ ,$$

defined on a one-particle Hilbert space $\mathcal{H}^1$. They obey certain canonical commutation and anti-commutation relations, called CCR and CAR, respectively. Apart from the standard notions, we introduce the corresponding self-dual algebras. This merely amounts to taking a different point of view. The only difference consists in singling out a different set of generators of these algebras, given by operator-valued functionals

$$f \mapsto B(f) \qquad \text{and} \qquad f \mapsto B^*(f) \ ,$$

defined on a larger space, called particle-hole space. In the fermion case, this space is again a Hilbert space, denoted by $\mathcal{L}$, while in the bosonic case it turns out to be a Krein space, denoted by $\mathcal{K}$. The advantage of this change of perspective is that the CCR and CAR can be written in a very compact way in terms of the generators $B(\cdot)$ and, more importantly, that homogeneous Bogoliubov transformations may be viewed as unitary transformations in $\mathcal{L}$, respectively $\mathcal{K}$. (We shall explain what we mean by unitarity in the latter case.) This observation allows us to develop the fermionic and bosonic theories in a very parallel fashion.

Furthermore, we introduce the concept of the truncated hierarchy of functionals associated to a state $\omega$, the properties of which are intimately related to the question of whether the state $\omega$ is quasi-free or not.

In Chapter 3 we introduce the notions of generalized density matrices, defined as a certain class of operators in the particle-hole space, and of quasi-free states in the context of both statistics. To any state $\omega$ we associate a generalized density matrix $\Gamma_\omega$, which essentially carries the information coded in its two-point functions. Since a quasi-free state is determined entirely by its two-point functions, it is not a surprise that there exists a 1:1-relation between generalized density matrices and quasi-free states. We prove this fact, assuming certain admissibility conditions. In the fermionic context the proof, taken from [8], makes use of the spectral theory of selfadjoint operators in the Hilbert space $\mathcal{L}$, as generalized density matrices may be represented in that way. In the bosonic case, however, generalized density matrices are represented by selfadjoint operators in the Krein space $\mathcal{K}$. We succeed in carrying over the proof from the fermionic context, by using the spectral theory of nonnegative operators in the Krein space sense. A short account on this theory and the proof of the central lemma is given in Appendix A. We believe that our proof is simpler and more constructive compared to a previous proof by Araki [2, 3].

Another object we pursue in this chapter is the development of the 'method of coherent states', again emphasizing the parallels between the two statistics. In order to achieve this goal, we use the technique of Grassmann variables to 'bosonify' the fermionic theory. The basic features of the Grassmann Algebra, together with a non-elementary bound on Gaussian Grassmann integrals, are presented in Appendix C. We use the coherent states approach to calculate the generating functional, i. e., a certain expectation value of a Gibbs state corresponding to a quadratic Hamiltonian. We use these relations to show, in the boson case, that Gibbs states associated to quadratic Hamiltonians are quasi-free.

Finally in Chapter 4, we turn to developing the HFB-Theory. First, we introduce (on a formal level) the type of models to be discussed. In particular, we investigate interactions given by pair-potentials $v$ defined on a three-dimensional torus $\Lambda$, allowing a decomposition of the type

$$v(x-y) = \int_0^\infty dr\, g(r) \int_\Lambda d^3z\, d_r(x) d_r(y) \quad , \qquad \forall\, x, y \in \Lambda,\ x \neq y\ ,$$

for suitable, nonnegative, measurable and bounded functions $g$ and $\{d_r\}_{r\in\mathbb{R}^+}$. This generalizes known decomposition formulae for pair-potentials on $\mathbb{R}^n$ [15, 20] in a straightforward way. We then use this decomposition formula to conveniently define the expectation value of the Hamiltonian $H$ in a quasi-free state $\omega$ in terms of its generalized density matrix $\Gamma_\omega$. In particular we exploit the fact that the above formula represents an interaction operator, possibly unbounded, as an integral of a tensor product of two bounded, nonnegative one-particle operators. It allows us to introduce a variational principle associated to $H$, without defining $H$ as a selfadjoint operator.

In Chapter 5 we finally turn to estimating the approximation error of HFB-Theory. In the fermion case we observe that, due to the Wick Theorem, the approximation error may be expressed as an expectation value of a quartic term in the particle generators and annihilators, normal-ordered in some generalized sense (we discuss this concept in Appendix B). Therefore, we estimate this term and obtain a correlation estimate, which generalizes the correlation estimate in [5]. We put this estimate to a test, by applying it to the Fermionic Jellium Model with periodic boundary conditions and Coulomb-Yukawa interaction, obtaining a similar estimate as [19].

In order to do the same for a bosonic model, one must first generalize the bosonic Wick Theorem to include the case of monomials in expressions of the type

$$a(f) + z \qquad \text{and} \qquad a^*(f) + z \ .$$

We present such a generalized Wick Theorem, which is proved in a straightforward manner. It turns out, however, that the approximation error is not just of the form of a normal-ordered quartic expectation value, as in the fermionic case. Nonetheless, as a first step, we derive a similar estimate as in the fermionic case. It is hoped that some day it may be helpful to adapt the method to the bosonic case and thereby facilitating an estimate of the ground state energy of the Bosonic Jellium Model by means of HFB-Theory.

At this point I would like to express my gratitude to all my colleagues in Berlin, who have been greatly supportive over the years. I am indebted to Prof. V. Bach and Prof. R. Seiler for the splendid cooperation and supervision and the possibility for numerous sojourns at Mainz University. Many thanks! Comments and answers by Prof. R. Wüst to many of my questions have been very valuable. Furthermore, I would like to thank Prof. P. Jonas and Dr. C. Trunk for their advice and help.

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# Chapter 1

# Foundations of Quantum Statistics

## 1.1 Second Quantization

### 1.1.1 Free Many-Particle Systems

In this subsection we introduce free many-particle systems, the word 'free' indicating that we view the particles as distinguishable. We use these systems exclusively for the purpose of defining the boson and fermion quantum many-particle systems.

For a beginning, we now construct the free $n$-particle system, where $n \in \mathbb{N}_0$ is arbitrary. Let $\mathcal{H}^1$ be a complex Hilbert space, called the <u>one-particle space</u>. We shall then, for any $n \in \mathbb{N}_0$, call the $n$-fold tensor product

$$\mathcal{H}^n := \underbrace{\mathcal{H}^1 \otimes \cdots \otimes \mathcal{H}^1}_{n\text{-factors}} \qquad \text{and} \qquad \mathcal{H}^0 := \mathbb{C} \tag{1.1}$$

the <u>free $n$-particle space</u>. To any one-particle observable, i. e., to any selfadjoint operator $A$ in $\mathcal{H}^1$ with dense domain $\mathcal{D}(A)$, we may associate an observable of the $n$-particle system. This $n$-particle observable is denoted by $\mathrm{d}\mathbf{G}_n(A)$ and is defined by:

$$\mathrm{d}\mathbf{G}_n(A) := A \otimes \mathbf{1} \otimes \cdots \otimes \mathbf{1} \;+\; \cdots \;+\; \mathbf{1} \otimes \cdots \otimes \mathbf{1} \otimes A \;, \qquad \mathrm{d}\mathbf{G}_0(A) := 0 \;.$$

Its domain is given by

$$\mathcal{D}\big(\,\mathrm{d}\mathbf{G}_n(A)\big) := \mathrm{span}\{\,\psi_1 \otimes \cdots \otimes \psi_n \mid \psi_1, \ldots, \psi_n \in \mathcal{D}(A)\,\} \;, \qquad \mathcal{D}\big(\,\mathrm{d}\mathbf{G}_0(A)\big) := \mathcal{H}^0 \;.$$

In order to construct a system with a variable number of particles, let us consider the linear space $\mathcal{H}^\infty$ of sequences of the form

$$\psi = \big\{\psi^{(n)}\big\}_{n \in \mathbb{N}_0} \;, \quad \text{with} \qquad \psi^{(n)} \in \mathcal{H}^n \;, \quad \forall\, n \in \mathbb{N}_0 \;. \tag{1.2}$$

We define the <u>free Fock space</u> as the subspace $\mathcal{F} \subseteq \mathcal{H}^\infty$ of those sequences, whose squared norms in each $\mathcal{H}^n$ sum up to a finite number. It then turns out that the series

$$\langle \psi \mid \phi \rangle_{\mathcal{F}} := \sum_{n=0}^{\infty} \Big\langle \psi^{(n)} \,\Big|\, \phi^{(n)} \Big\rangle_{\mathcal{H}^n} \tag{1.3}$$

is absolutely convergent, for any $\psi, \phi \in \mathcal{F}$, and defines a scalar product. Furthermore, $\mathcal{F}$ is complete with respect to the induced norm and is therefore a Hilbert space. We have thus accomplished the aim of defining the state space of a system of arbitrarily many-particles. The following special element of this space

$$\Omega := \{1, 0, 0, \dots\} \tag{1.4}$$

is called the vacuum.

As a next step, we associate to a one-particle observable $A$ an observable $\mathrm{d}\mathbf{G}(A)$ on the free Fock space $\mathcal{F}$. This new observable, to be defined, is called the second Quantization of $A$. To that end, we shall from now on regard the spaces $\mathcal{H}^0, \mathcal{H}^1, \dots$ as subspaces of $\mathcal{F}$, implying the embedding:

$$\psi^{(n)} \in \mathcal{H}^n \;\mapsto\; \{\psi^{(m)}\}_{m \in \mathbb{N}_0} , \qquad \text{where} \qquad \psi^{(m)} = 0 , \qquad \forall\, n \neq m . \tag{1.5}$$

Furthermore, these subspaces are obviously pairwise orthogonal, and hence it makes sense to write $\mathcal{F}$ as an infinite, orthogonal sum

$$\mathcal{F} \;=\; \bigoplus_{n=0}^{\infty} \mathcal{H}^n . \tag{1.6}$$

We introduce the subspace of finite vectors

$$F \;:=\; \Big\{\psi \in \mathcal{F} \;\big|\; \psi^{(n)} = 0 \quad \forall\, n > n_0,\ \text{for some } n_0 \in \mathbb{N}\Big\} . \tag{1.7}$$

**Definition 1.1.** *For any densly defined, selfadjoint operator $A$ in $\mathcal{H}^1$, we define a symmetric operator $G$ in $\mathcal{F}$, by setting*

$$G{\restriction}_{\mathcal{H}^n} \;:=\; \mathrm{d}\mathbf{G}_n(A) \quad , \qquad \forall\, n \in \mathbb{N}_0 , \tag{1.8}$$

*and extending it by linearity to the dense domain*

$$D := \Big\{\psi \in F \;\big|\; \psi^{(n)} \in \mathcal{D}\big(\mathrm{d}\mathbf{G}_n(A)\big) \;\; \forall\, n \in \mathbb{N}_0\Big\} . \tag{1.9}$$

*The operator $\mathrm{d}\mathbf{G}(A)$, obtained from $G$ by closing it in the graph norm, is called the second quantization of $A$.*

**Theorem 1.2.** *The operator $\mathrm{d}\mathbf{G}(A)$ is selfadjoint and $D$ is a core of $A$.*

*Proof:* By Nelson's analytic vectors theorem (see, e. g., [26]) it suffices to show that $D$ contains a total set of analytic vectors. We point out that $A$, being selfadjoint, automatically possesses such a set $C_A$ of analytic vectors. Correspondingly, we consider the family of vectors

$$C := \{\, \psi \mid \psi = \varphi_1 \otimes \cdots \otimes \varphi_n \in \mathcal{H}^n, \;\; \text{for some } n \in \mathbb{N} \text{ and } \varphi_1, \dots, \varphi_n \in C_A \,\} . \tag{1.10}$$

(Recall the embedding given in relation (1.5).) Obviously, the family $C$ is total and is contained in the domain of $(G{\restriction}_D)^k$, for any $k \in \mathbb{N}$. For any $\psi \in C$ with $\psi = \psi^{(n)} =$

$\varphi_1 \otimes \cdots \otimes \varphi_n$, we have

$$\begin{aligned}
\sum_{k=0}^{\infty} \frac{1}{k!} \left\| G^k \psi \right\|_{\mathcal{F}} &= \sum_{k=0}^{\infty} \frac{1}{k!} \left\| \mathrm{d}\mathbf{G}_n(A)^k \varphi_1 \otimes \cdots \otimes \varphi_n \right\|_{\mathcal{H}^n} \\
&\leq \sum_{k=0}^{\infty} \frac{1}{k!} \sum_{j_1+\cdots+j_n=k} \frac{k!}{j_1! \cdots j_n!} \| A^{j_1} \varphi_1 \|_{\mathcal{H}^1} \cdots \| A^{j_1} \varphi_n \|_{\mathcal{H}^1} \\
&= \left( \sum_{j=0}^{\infty} \frac{1}{j!} \| A^j \varphi_1 \|_{\mathcal{H}^1} \right) \cdots \left( \sum_{j=0}^{\infty} \frac{1}{j!} \| A^j \varphi_n \|_{\mathcal{H}^1} \right) . \qquad (1.11)
\end{aligned}$$

Since $\varphi_1, \dots, \varphi_n$ are analytic vectors of $A$, it follows that the right hand side is finite. Hence, we have found a total family $C$ of analytic vectors of $G$ and have thereby proved the theorem. $\square$

In particular the operator given by $\mathbf{n} := \mathrm{d}\mathbf{G}(\mathbf{1})$ is selfadjoint (and nonnegative). We shall call $\mathbf{n}$ the particle number operator. As can easily be verified, $\mathbf{n}$ can be reexpressed by

$$\mathbf{n}\,\psi = \left\{ n \cdot \psi^{(n)} \right\}_{n \in \mathbb{N}_0} , \quad \text{where} \quad \mathcal{D}(\mathbf{n}) = \left\{ \psi \in \mathcal{F} \;\middle|\; \sum_{n=0}^{\infty} n^2 \left\| \psi^{(n)} \right\|^2 < \infty \right\} . \qquad (1.12)$$

Another way of assigning operators in Fock space to one-particle operators in $\mathcal{H}^1$ is given by the definition:

$$\mathbf{G}_n(U) := \underbrace{U \otimes \cdots \otimes U}_{n\text{-factors}} , \qquad \text{for any operator } U : \mathcal{H}^1 \to \mathcal{H}^1 . \qquad (1.13)$$

This defines an operator on $F$ by linearity. If only $\| U \| \leq 1$, this operator is bounded and thus extends to a unique bounded operator defined on the whole of $\mathcal{F}$. In particular, the functor $\mathbf{G}$ maps unitary operators to unitary operators. Given a one-particle observable $A$, we have

$$\mathbf{G}\big(e^{iA}\big) = e^{i\,\mathrm{d}\mathbf{G}(A)} . \qquad (1.14)$$

If, in turn, we are given some complete orthonormal system $\{f_j\}_{j\in J}$ in $\mathcal{H}^1$ and an orthogonal projection $P_{J'}$ in $\mathcal{H}^1$ onto the span of $\{f_j\}_{j\in J'}$ for some $J' \subseteq J$, it follows that $\mathbf{G}(P_{J'})$ is itself an orthogonal projection in $\mathcal{F}$ and

$$\mathbf{G}(P_{J'}) f_{j_1} \otimes \cdots \otimes f_{j_N} = \begin{cases} f_{j_1} \otimes \cdots \otimes f_{j_N} & \text{if } j_1, \dots, j_N \in J' \\ 0 & \text{else} \end{cases} , \qquad (1.15)$$

for all $j_1, \dots, j_N \in J$.

The objects we introduce next serve exclusively the purpose of defining their bosonic and fermionic counterparts. The following relations define, again by linearity, operators from $\mathcal{H}^n$ to $\mathcal{H}^{n-1}$ and $\mathcal{H}^{n+1}$, respectively:

$$a_\circ(f)\psi_1 \otimes \cdots \otimes \psi_n \;:=\; \sqrt{n}\,\langle f \,|\, \psi_1 \rangle \cdot \psi_2 \otimes \cdots \otimes \psi_n , \qquad (1.16)$$

$$a_\circ^*(f)\psi_1 \otimes \cdots \otimes \psi_n \;:=\; \sqrt{n+1} \cdot f \otimes \psi_1 \otimes \cdots \otimes \psi_n , \qquad (1.17)$$

for any $n \in \mathbb{N}$, $f \in \mathcal{H}^1$ and all $\psi_1, \cdots, \psi_n \in \mathcal{H}^1$. Furthermore, we set

$$a_\circ(f)\Omega := 0 \qquad \text{and} \qquad a_\circ^*(f)\Omega := f \; . \tag{1.18}$$

Obviously, $a_\circ(\cdot)$ and $a_\circ^*(\cdot)$ can be viewed as densly defined operators in $\mathcal{F}$, which we shall call free particle annihilation operator and free particle creation operator, respectively. By the following theorem, these can be defined as closed operators on the domain

$$\mathcal{D}\big(a_\circ^\tau(f)\big) := \mathcal{D}(\sqrt{\mathbf{n}}) \qquad \text{for} \qquad \tau \in \{\varnothing, *\} \quad \text{and} \quad f \in \mathcal{H}^1 \; . \tag{1.19}$$

**Theorem 1.3.** *For any $n \in \mathbb{N}_0$, the restrictions of $a_\circ(f)$ and $a_\circ^*(f)$ to the $n$-particle space are bounded, for any $f \in \mathcal{H}^1$, and fulfill the following relations:*

$$\| \, a_\circ(f){\restriction}_{\mathcal{H}^n} \| = \sqrt{n} \cdot \| \, f \, \| \qquad \textit{and} \qquad \| \, a_\circ^*(f){\restriction}_{\mathcal{H}^n} \| = \sqrt{n+1} \cdot \| \, f \, \| \; . \tag{1.20}$$

*Proof:* Let $\{\varphi_j\}_{j\in J}$ be an orthonormal set of vectors in $\mathcal{H}^1$. For arbitrary $n \in \mathbb{N}$, let $\psi \in \mathcal{H}^n$ be given by

$$\psi = \sum_{j_1,\ldots,j_n \in J} c_{j_1,\ldots,j_n} \varphi_{j_1} \otimes \cdots \otimes \varphi_{j_n} \qquad \text{and} \qquad \sum_{j_1,\ldots,j_n \in J} |\, c_{j_1,\ldots,j_n} |^2 = 1 \; . \tag{1.21}$$

This last condition is equivalent to $\| \, \psi \, \| = 1$. We now compute

$$\begin{aligned} \| \, a_\circ(f)\psi \, \|^2 &= n \left\| \sum_{j_1,\ldots,j_n \in J} c_{j_1,\ldots,j_n} \langle f \,|\, \varphi_{j_1} \rangle \, \varphi_2 \otimes \cdots \otimes \varphi_{j_n} \right\|^2 \\ &= n \sum_{j_2,\ldots,j_n \in J} \left| \sum_{j_1 \in J} c_{j_1,\ldots,j_n} \langle f \,|\, \varphi_{j_1} \rangle \right|^2 \\ &\le n \, \| \, f \, \|^2 \sum_{j_1,\ldots,j_n \in J} |\, c_{j_1,\ldots,j_n} |^2 = n \, \| \, f \, \|^2 \; . \end{aligned} \tag{1.22}$$

The optimality of this inequality follows from the observation that, for all normalized vectors $\varphi_1, \ldots, \varphi_n \in \mathcal{H}^1$,

$$\| \, a_\circ(\varphi)\varphi_1 \otimes \cdots \otimes \varphi_n \, \| = \sqrt{n} \; . \tag{1.23}$$

The proof of the second claim is completely analogous. □

For any $f \in \mathcal{H}^1$, the following adjointness relation holds:

$$\langle a_\circ(f)\psi \,|\, \phi \rangle_{\mathcal{F}} = \langle \psi \,|\, a_\circ^*(f)\phi \rangle_{\mathcal{F}} \quad , \qquad \forall \; \psi, \phi \in \mathcal{D}(\sqrt{\mathbf{n}}) \tag{1.24}$$

*Proof:* Since $a_\circ(f)$ is closed and by the linearity properties of the scalar product, it suffices to prove relation (1.24) in the case

$$\psi = \psi_1 \otimes \cdots \otimes \psi_{n+1} \in \mathcal{H}^{n+1} \qquad \text{and} \qquad \phi = \phi_1 \otimes \cdots \otimes \phi_n \in \mathcal{H}^n \; , \tag{1.25}$$

for arbitrary $\psi_1, \ldots, \psi_{n+1}, \phi_1, \ldots, \phi_n \in \mathcal{H}^1$. In this case, we have

$$\begin{aligned} \langle a_\circ(f)\psi \,|\, \phi \rangle_{\mathcal{H}^n} &= \sqrt{n} \, \langle \psi_1 \,|\, f \rangle_{\mathcal{H}^1} \cdot \langle \psi_2 \otimes \cdots \otimes \psi_{n+1} \,|\, \phi_1 \otimes \cdots \otimes \phi_n \rangle_{\mathcal{H}^n} \\ &= \sqrt{n} \, \langle \psi_1 \otimes \cdots \otimes \psi_{n+1} \,|\, f \otimes \phi_1 \otimes \cdots \otimes \phi_n \rangle_{\mathcal{H}^{n+1}} \\ &= \langle \psi \,|\, a_\circ^*(f)\phi \rangle_{\mathcal{H}^{n+1}} \; . \end{aligned} \tag{1.26}$$

□

This also shows that the algebra generated by the particle annihilation and particle creation operators is a $*$-algebra.

### 1.1.2 Bosonic Many-Particle Systems, CCR and Weyl Algebra

In this section we construct the boson Fock space as the totally symmetric subspace of the free Fock space we just defined, by introducing the corresponding projection in the following way: By linearity we define an operator $\mathcal{S}_+$ on $F \subseteq \mathcal{F}$, by

$$\mathcal{S}_+ \psi_1 \otimes \cdots \otimes \psi_n := \frac{1}{n!} \sum_{\pi \in S_n} \psi_{\pi(1)} \otimes \cdots \otimes \psi_{\pi(n)} \quad , \qquad \forall\, \psi_1, \ldots, \psi_n \in \mathcal{H}^1 \ . \tag{1.27}$$

This operator is symmetric, bounded and idempotent and thus completely determines a selfadjoint projection $\mathcal{S}_+ : \mathcal{F} \to \mathcal{F}$. With the aid of this projection we now define the boson Fock space $\mathcal{F}_+$, its subspace of finite vectors $F_+$ and also its $n$-particle subspaces $\mathcal{H}^n_+$ by

$$\mathcal{F}_+ := \mathcal{S}_+ \mathcal{F} \ , \qquad F_+ := \mathcal{S}_+ F \ , \qquad \mathcal{H}^n_+ := \mathcal{S}_+ \mathcal{H}^n \ . \tag{1.28}$$

For any $f \in \mathcal{H}^1$, we introduce the boson particle annihilation operator and the boson particle creation operator by

$$a(f) := \mathcal{S}_+ a_\circ(f) \mathcal{S}_+ \qquad \text{and} \qquad a^*(f) := \mathcal{S}_+ a^*_\circ(f) \mathcal{S}_+ \ . \tag{1.29}$$

The domain of these operators, seen as operators in $\mathcal{F}_+$, is obviously given by $\mathcal{S}_+ \mathcal{D}(\sqrt{\mathbf{n}})$. Furthermore, $F_+$ is an invariant subspace of both. This last fact guarantees that any polynomial of such operators is at least defined on $F_+$. Moreover, they obey, for all $f, g \in \mathcal{H}^1$, the following canonical commutation relations (CCR):

$$[a(f), a^*(g)]\restriction_{F_+} = \langle f \,|\, g \rangle \cdot \mathbf{1}\restriction_{F_+} \ , \qquad [a(f), a(g)]\restriction_{F_+} = [a^*(f), a^*(g)]\restriction_{F_+} = \mathbf{0}\restriction_{F_+} \ , \tag{1.30}$$

with $[A, B] := AB - BA$ for any two operators $A$ and $B$ in $\mathcal{F}_+$.

*Proof:* It suffices to prove the commutation relations on elements of the form

$$\psi = \mathcal{S}_+ \psi_1 \otimes \cdots \otimes \psi_n \in \mathcal{H}^n_+ \ , \tag{1.31}$$

for some $\psi_1, \ldots, \psi_n \in \mathcal{H}^1$. First, let us observe that we have, for any $f \in \mathcal{H}^1$ and any such $\psi$,

$$a^*(f) \mathcal{S}_+ \psi_1 \otimes \cdots \otimes \psi_n = \sqrt{n+1}\, \mathcal{S}_+ f \otimes \psi_1 \otimes \cdots \otimes \psi_n \tag{1.32a}$$

$$a(f) \mathcal{S}_+ \psi_1 \otimes \cdots \otimes \psi_n = \frac{1}{\sqrt{n}} \sum_{j=1}^{n} \langle f \,|\, \psi_j \rangle\, \mathcal{S}_+ \psi_1 \otimes \cdots \otimes \widehat{\psi_j} \otimes \cdots \otimes \psi_n \ . \tag{1.32b}$$

By the notation $\widehat{\psi_j}$ we indicate that the corresponding factor $\psi_j$ is absent in the above tensor product. With the help of these two relations we obtain, for all $f, g \in \mathcal{H}^1$, on the one hand

$$\begin{aligned} a(f) a^*(g) \mathcal{S}_+ \psi_1 \otimes \cdots \otimes \psi_n &= \sqrt{n+1} \cdot a(f) \mathcal{S}_+ g \otimes \psi_1 \otimes \cdots \otimes \psi_n \\ &= \langle f \,|\, g \rangle\, \mathcal{S}_+ \psi_1 \otimes \cdots \otimes \psi_n + \sum_{j=1}^{n} \langle f \,|\, \psi_j \rangle\, \mathcal{S}_+ g \otimes \psi_1 \otimes \cdots \otimes \widehat{\psi_j} \otimes \cdots \otimes \psi_n \end{aligned}$$

and on the other hand

$$\begin{aligned} a^*(g)a(f)\mathcal{S}_+\psi_1 \otimes \cdots \otimes \psi_n &= \frac{1}{\sqrt{n}} \sum_{j=1}^{n} \langle f \,|\, \psi_j \rangle \, a^*(g)\mathcal{S}_+\psi_1 \otimes \cdots \otimes \widehat{\psi_j} \otimes \cdots \otimes \psi_n \\ &= \sum_{j=1}^{n} \langle f \,|\, \psi_j \rangle \, \mathcal{S}_+ g \otimes \psi_1 \otimes \cdots \otimes \widehat{\psi_j} \otimes \cdots \otimes \psi_n \; . \end{aligned} \tag{1.33}$$

This proves the first of the three commutation relations claimed. The second and third relation are obvious. □

The algebra $\mathcal{A}_{\mathrm{ccr}}(\mathcal{H}^1)$ of polynomials in the operators $\{a(f)\}_{f\in\mathcal{H}^1}$ and $\{a^*(f)\}_{f\in\mathcal{H}^1}$ is called the CCR Algebra over $\mathcal{H}^1$. Due to the adjointness relation (1.24) we have for all $f \in \mathcal{H}^1$

$$a^*(f) \subseteq (a(f))^* \qquad \text{and} \qquad a(f) \subseteq (a^*(f))^* \; . \tag{1.34}$$

In view of relation (1.23) and because of the fact that the $n$-fold tensor product of any normalized $\varphi \in \mathcal{H}^1$ with itself is an element of $\mathcal{H}^n_+ \subseteq \mathcal{F}_+$, we deduce that the operators $a(f)$ and $a^*(f)$ are unbounded in any nontrivial case. Therefore, they do generally *not* define a $C^*$-algebra. However, it can be shown that

$$\big(a(f)\big)^* = a^*(f) \qquad \text{and} \qquad \big(a^*(f)\big)^* = a(f) \quad , \qquad \forall\, f \in \mathcal{H}^1 \; . \tag{1.35}$$

We remind the reader that $a^*(f)$ and $a(f)$ are both defined on $\mathcal{S}_+\mathcal{D}(\sqrt{\mathbf{n}})$, for all $f \in \mathcal{H}^1$.

The technical difficulties coming along with the unboundedness of the boson particle annihilation and creation operators can partly be overcome with the introduction of the Weyl Operators. In order to proceed along these lines, we first introduce the boson field, denoted by $\Phi(\cdot)$ and defined by

$$\Phi(f) := \tfrac{1}{\sqrt{2}}\overline{\big(\, a(f) + a^*(f) \,\big)} \quad , \qquad \forall\, f \in \mathcal{H}^1 \; . \tag{1.36}$$

The question of well-definedness and the properties of these objects are addressed in the following theorem.

**Theorem 1.4.**

1. *The operator $a(f) + a^*(f)$ is essentially selfadjoint on $\mathcal{D}(\sqrt{\mathbf{n}})$, for any $f \in \mathcal{H}^1$.*
2. *The span of $\{\Phi(f_1)\cdots\Phi(f_n)\Omega \mid f_1,\ldots,f_n \in \mathcal{H}^1, n \in \mathbb{N}_0\}$ is a dense subset of $F_+$.*
3. *For any $f, g \in \mathcal{H}^1$ the following commutation relation[1] holds true:*

$$[\Phi(f), \Phi(g)]\restriction_{F_+} = i \,\mathrm{Im}\, \langle f \,|\, g \rangle \, \mathbf{1}\restriction_{F_+} \tag{1.37}$$

*Proof:* (1): Since the operator $A := a(f) + a^*(f)$ is defined on the dense set $F_+$ and is symmetric, it is also closable. As in the proof of Theorem 1.2, it therefore suffices to show

[1]It can be shown that this identity also holds on $\mathcal{D}(\sqrt{\mathbf{n}})$

that there exists a total set of analytic vectors for $A$. As we have already pointed out, for any $m \in \mathbb{N}$, we have $F_+ \subseteq \mathcal{D}(A^m)$. It is thus also true, that

$$\| A^m \psi \| \leq \sum_{\tau_1,\ldots,\tau_m \in \{\varnothing,*\}} \| a^{\tau_1}(f) \cdots a^{\tau_m}(f) \psi \| \ \leq\ 2^m \sqrt{(m+n+1)!}\, \| \psi \| \, \| f \|^m \ , \quad (1.38)$$

for any $n \in \mathbb{N}_0$ and all $\psi \in \mathcal{H}^n_+$. The symbol $\varnothing$ is used to represent 'the absence of a star', namely we denote $a^{\varnothing}(f) = a(f)$. In the last estimate above, we have used

$$\| a^{\tau}(f)\psi \| \ \leq\ \sqrt{1+n}\, \| \psi \| \, \| f \| \quad , \qquad \forall\ \tau \in \{\varnothing, *\} \ , \quad (1.39)$$

being a consequence of Theorem 1.3. We have therefore shown that, for sufficiently small $t > 0$,

$$\sum_{m=0}^{\infty} \frac{1}{m!} \| (tA)^m \psi \| \ \leq\ \| \psi \| \sum_{m=0}^{\infty} \frac{\sqrt{(n+m+1)!}}{m!} \| 2f \|^m t^m \ <\ \infty \ . \quad (1.40)$$

Stirling's formula can be used to show that the coefficients $\frac{\sqrt{(n+m+1)!}}{m!}$ are bounded.

(2): Note that the span of the fields appearing in the claim is equal to the span of

$$\left\{ a^*(f_1) \cdots a^*(f_n)\Omega \mid f_1, \ldots, f_n \in \mathcal{H}^1, n \in \mathbb{N}_0 \right\} \quad (1.41)$$

and that by relation (1.32a) it holds

$$a^*(f_1) \cdots a^*(f_n)\Omega = \sqrt{n!} \cdot \mathcal{S}_+ f_1 \otimes \cdots \otimes f_n \ . \quad (1.42)$$

for all $n \in \mathbb{N}$ and $f_1, \ldots, f_n \in \mathcal{H}^1$.

(3): To prove the third claim use the CCR. □

We now introduce the Weyl Algebra. We define

$$W(f) \ :=\ \exp\big(i\Phi(f)\big) \quad , \qquad \forall\ f \in \mathcal{H}^1 \ , \quad (1.43)$$

the right hand side of this relation being given by the spectral theorem. The closure in the operator norm of the algebra generated by $\{W(f)\}_{f \in \mathcal{H}^1}$ is called the Weyl Algebra over $\mathcal{H}^1$, denoted in shorthand notation by $\mathcal{W}\left(\mathcal{H}^1\right)$. In fact $\mathcal{W}\left(\mathcal{H}^1\right)$ coincides with the $C^*$-algebra $\mathcal{B}(\mathcal{H}^1)$. The boson fields obey the following simple transformation rule under the action of Weyl operators:

**Theorem 1.5.** *The domain of $\Phi(g)$ is, for any $g \in \mathcal{H}^1$, invariant under the action of $W(f)$, for arbitrary $f \in \mathcal{H}^1$. Furthermore, we have*

$$W(f)\Phi(g)W(f)^* = \Phi(g) - \operatorname{Im} \langle f \,|\, g \rangle \cdot \mathbf{1} \ . \quad (1.44)$$

*Proof:* For any $\psi \in F_+$ and arbitrary $K \in \mathbb{N}$, we obtain from (1.37) the relation

$$\Phi(g) \sum_{k=0}^{K} \frac{(-i)^k}{k!} \Phi(f)^k \psi = \left\{ \sum_{k=0}^{K} \frac{(-i)^k}{k!} \Phi(f)^k \Phi(g) - \sum_{k=0}^{K-1} \frac{(-i)^k}{k!} \Phi(f)^k \operatorname{Im} \langle f \,|\, g \rangle \right\} \psi \ . \quad (1.45)$$

By the fact that both $\psi$ and $\Phi(g)\psi$ are analytic vectors of $\Phi(f)$ and because $\Phi(g)$ is closed, we deduce, for any $\psi \in F_+$:

$$\Phi(g)W(f)^*\psi = W(f)^*\big\{\Phi(g) - \mathrm{Im}\,\langle f \,|\, g\rangle\,\big\}\psi \ . \tag{1.46}$$

The equality of the Weyl operator with its power-series on the analytic vector $\psi$ readily follows from Stone's theorem. It remains to prove that this relation also holds for arbitrary $\tilde{\psi} \in \mathcal{D}\big(\Phi(g)\big)$. We remark that the last equality implies

$$\begin{aligned} &\big\|\, \Phi(g)W(f)^*(\psi - \psi')\,\big\| \\ &\qquad \leq \big\|\, \Phi(g)(\psi - \psi')\,\big\| + |\,\mathrm{Im}\,\langle f \,|\, g\rangle\,|\,\big\|\, \psi - \psi'\,\big\| \quad , \qquad \forall\, \psi, \psi' \in F_+ \ . \end{aligned} \tag{1.47}$$

Since $\mathcal{D}\big(\Phi(g)\big)$ is the closure of $F_+$ in the graph norm of $\Phi(g)$, for any $\tilde{\psi} \in \mathcal{D}\big(\Phi(g)\big)$ there exists a sequence $\{\psi_n\}_{n\in\mathbb{N}}$ of finite vectors with the following convergence properties:

$$\psi_n \xrightarrow{n\to\infty} \tilde{\psi} \qquad \text{and} \qquad \Phi(g)\psi_n \xrightarrow{n\to\infty} \Phi(g)\tilde{\psi} \ . \tag{1.48}$$

From the above estimate, we see that $\Phi(g)W(f)^*\psi_n$ converges. Hence $\psi_n \to \tilde{\psi}$ converges in the graph norm of $\Phi(g)W(f)^*$ and by the closedness of $\Phi(g)$ we have $W(f)^*\psi \in \mathcal{D}(\Phi(g))$ and relation (1.46) holds also for arbitrary $\tilde{\psi} \in \mathcal{D}(\Phi(g))$. □

**Theorem 1.6.** *The following* <u>*concatenation relation*</u> *holds true, for any two elements $f$ and $g$ of the one-particle space $\mathcal{H}^1$:*

$$W(f)W(g) = e^{-\frac{i}{2}\,\mathrm{Im}\langle f|\,g\,\rangle}\,W(f+g) \ . \tag{1.49}$$

*Proof:* By Theorem 1.5 the domains of all fields are invariant under the action of any Weyl operator. Moreover $F_+$ is contained in the domain of any field and relation (1.46) holds. This implies, for all $\psi \in F_+$, $f, g \in \mathcal{H}^1$ and $t$ in $\mathbb{R}$:

$$\begin{aligned} \frac{d}{dt} W(tf)W(tg)W\big(t(f+g)\big)^*\psi &= W(tf)\,[i\Phi(f), W(tg)]\,W\big(t(f+g)\big)^*\psi \\ &= -it\,\mathrm{Im}\,\langle f \,|\, g\rangle\, W(tf)W(tg)W\big(t(f+g)\big)^*\psi \ . \end{aligned} \tag{1.50}$$

Since all Weyl operators are unimodular, the claim follows. □

### 1.1.3 The Self-Dual CCR Algebra

The self-dual CCR Algebra was originally introduced by Araki [2, 3]. It is defined over a linear vector space, which is actually a Krein space. We summarize the fundamental notions of linear operators in Krein spaces in Appendix A.

We consider the linear space $\mathcal{K}$ given by column vectors with two entries from $\mathcal{H}^1$, i. e.,

$$\mathcal{K} \ := \ \left\{ \begin{pmatrix} f^+ \\ f^- \end{pmatrix} \,\Big|\, f^\pm \in \mathcal{H}^1 \right\} \ , \tag{1.51}$$

where we agree to define the sum of two vectors and the exterior product in the standard way. For any $f \in \mathcal{K}$, we denote the first entry by $f^+$, the second entry by $f^-$, thus defining the projections $f \mapsto f^{\pm}$ from $\mathcal{K}$ into $\mathcal{H}^1$. Together with the inner product $[\cdot\,|\,\cdot]$ on $\mathcal{K}$ given by

$$[f\,|\,g] := \langle f^+\,|\,g^+\rangle_{\mathcal{H}^1} - \langle f^-\,|\,g^-\rangle_{\mathcal{H}^1} \quad , \qquad \forall\, f,g \in \mathcal{K}\ , \tag{1.52}$$

this space is a Krein space, admitting the following <u>fundamental decomposition</u>, in the sense of Definition A.2,

$$\mathcal{K} = \mathcal{K}_+ {}^{[+]}\, \mathcal{K}_- \tag{1.53a}$$

with

$$\mathcal{K}_+ := \left\{ \begin{pmatrix} f \\ 0 \end{pmatrix} \,\middle|\, f \in \mathcal{H}^1 \right\} \qquad \text{and} \qquad \mathcal{K}_- := \left\{ \begin{pmatrix} 0 \\ f \end{pmatrix} \,\middle|\, f \in \mathcal{H}^1 \right\}\ . \tag{1.53b}$$

Here we have denoted by $\langle\cdot\,|\,\cdot\rangle_{\mathcal{H}^1}$ the scalar product on the Hilbert space $\mathcal{H}^1$. From now on, we shall drop the subscript $\mathcal{H}^1$, whenever it is clear from the context which scalar product is meant.

Additionally we assume that we are given a <u>conjugation</u> $\tau : \mathcal{K} \to \mathcal{K}$ defined in the following way: Suppose that $\mathcal{H}^1$ is equipped with an antiunitary involution

$$\overline{(\,\cdot\,)} : \mathcal{H}^1 \to \mathcal{H}^1, \quad f \ \mapsto\ \bar{f}\ , \tag{1.54}$$

satisfying

$$\langle \bar{f}\,|\,\bar{g}\rangle = \overline{\langle f\,|\,g\rangle} = \langle g\,|\,f\rangle \quad , \qquad \forall\, f,g \in \mathcal{H}^1\ . \tag{1.55}$$

If, for example, $\mathcal{H}^1$ is an $L^2$ space of complex-valued functions, such a conjugation on $\mathcal{H}^1$ could then given by pointwise conjugation in the sense of complex numbers of the elements of $\mathcal{H}^1$. We then define the conjugation $\tau : \mathcal{K} \to \mathcal{K}$ by

$$\tau \begin{pmatrix} f^+ \\ f^- \end{pmatrix} := \begin{pmatrix} \bar{f}^- \\ \bar{f}^+ \end{pmatrix} \quad , \qquad \forall\ f = \begin{pmatrix} f^+ \\ f^- \end{pmatrix} \in \mathcal{K}\ . \tag{1.56}$$

For any fundamental decomposition $\mathcal{K} = \tilde{\mathcal{K}}_+ {}^{[+]}\, \tilde{\mathcal{K}}_-$ (see Definition A.2), possibly different from (1.53), we now introduce the notion of self-duality. We say such a decomposition is <u>self-dual</u> if it satisfies

$$\tau\tilde{\mathcal{K}}_\pm = \tilde{\mathcal{K}}_\mp\ . \tag{1.57}$$

It is obvious that the fundamental decomposition (1.53) is self-dual. The conjugation $\tau$ satisfies the following compatibility condition with respect to the inner product

$$[\tau f\,|\,\tau g] = -\,[g\,|\,f] \quad , \qquad \forall\ f,g \in \mathcal{K}\ . \tag{1.58}$$

For any $f \in \mathcal{K}$, we single out two elements $B(f)$ and $B^*(f)$ of the CCR Algebra, by setting

$$B(f) := a^*(f^+) + a(\bar{f}^-) \qquad \text{and} \qquad B^*(f) := a(f^+) + a^*(\bar{f}^-)\ . \tag{1.59}$$

Obviously, we have chosen these two algebra elements to be adjoint to each others and we have

$$B^*(f) = \big(B(f)\big)^* = B(\tau f) \quad , \qquad \forall\ f \in \mathcal{K}\ . \tag{1.60}$$

The relevance of the concepts we introduce above is now becoming clear. The Krein space $\mathcal{K}$ is to be interpreted as a particle-hole space and the fundamental decomposition (1.53) corresponds to a certain kind of quasi-particles. The conjugation $\tau$ is to be viewed as a particle-hole duality. Due to the assumption of self-duality, all fundamental decompositions admit such an interpretation.

The linear functionals $B(\cdot)$, with values in the CCR Algebra, allow us to treat particle annihilation and particle creation operators on an equal footing and thus to rewrite the CCR in a very condensed form:

$$[B^*(f), B(g)]\restriction_{F_+} = [f \mid g]\, \mathbf{1}\restriction_{F_+} \quad , \qquad \forall\, f, g \in \mathcal{K} \ . \tag{1.61}$$

Even though the $*$-algebra generated by the functionals $B(\cdot)$ is no other algebra than the CCR Algebra, it is in this context common to term it the self-dual CCR Algebra over $\mathcal{H}^1$.

Independently of any fundamental decomposition and depending only on the choice of $\tau$, there is one particular real subspace of $\mathcal{K}$, given by

$$\mathcal{K}_{\mathbb{R}} := \{f \in \mathcal{K} \mid \tau f = f\} = \left\{ \begin{pmatrix} f \\ \bar{f} \end{pmatrix} \;\middle|\; f \in \mathcal{H}^1 \right\} \ . \tag{1.62}$$

Evidently there is a 1:1-correspondence between $\mathcal{K}_{\mathbb{R}}$ and $\mathcal{H}^1$ and we can therefore associate to each element of $\mathcal{H}^1$ a unique element of $\mathcal{K}_{\mathbb{R}}$ and vice-versa, by the following map $\rho$

$$\rho : \mathcal{H}^1 \to \mathcal{K}_{\mathbb{R}} \ , \quad \text{with} \qquad \rho(g) := \frac{1}{\sqrt{2}} \begin{pmatrix} g \\ \bar{g} \end{pmatrix} \ . \tag{1.63}$$

It is, however, important to keep in mind that $\rho$ is *not* complex linear.

In accordance with the interpretation of $\mathcal{K}$ as a particle-hole space, we may understand homogeneous Bogoliubov transformations (see Chapter 2) of the CCR Algebra as operators $w : \mathcal{K} \to \mathcal{K}$ obeying the following restrictions:

$$w^{[*]} w = w w^{[*]} = \mathbf{1} \qquad \text{and} \qquad \tau w \tau = w \ . \tag{1.64}$$

The operator $w^{[*]}$, defined in Appendix A, is the adjoint of $w$ with respect to the inner product $[\cdot \mid \cdot]$. We give a short review of the concept of Bogoliubov transformations in Chapter 2. The first of the two restrictions means just that $w$ is a unitary operator with respect to the inner product $[\cdot \mid \cdot]$ and thus ensures that the commutation relation (1.61) remain invariant under $w$. The second restriction means that particles and holes should transform in a dual way. It is thus clear that, $w$ being any homogeneous Bogoliubov transformation, the subspaces $\tilde{\mathcal{K}}_+, \tilde{\mathcal{K}}_- \subseteq \mathcal{K}$, given by $\tilde{\mathcal{K}}_\pm := w\mathcal{K}_\pm$, are Hilbert spaces with respect to the scalar products $\pm[\cdot \mid \cdot]\restriction_{\tilde{\mathcal{K}}_\pm}$. It also follows that the decomposition

$$\mathcal{K} = \tilde{\mathcal{K}}_+ {}^{[+]}\, \tilde{\mathcal{K}}_- \tag{1.65}$$

is again a self-dual fundamental decomposition. We prove this statements in Theorem A.4. Conversely, if we are given a fundamental decomposition (1.65) then the subspaces $\tilde{\mathcal{K}}_\pm$ and $\mathcal{K}_\pm$ are unitarily equivalent (as Hilbert spaces, of course), see Section I in [22]. Now, if $w_+ : \mathcal{K}_+ \to \tilde{\mathcal{K}}_+$ is unitary in the Hilbert space sense, so is $w_- := \tau w_+ \tau$ and

$$w f := w_+ f_+ + w_- f_- \quad , \qquad \forall\, f \in \mathcal{K} \tag{1.66}$$

defines a homogeneous Bogoliubov transformation $w$. Here, we have used the following notation

$$f_+ := \begin{pmatrix} f^+ \\ 0 \end{pmatrix} \qquad \text{and} \qquad f_- := \begin{pmatrix} 0 \\ f^- \end{pmatrix} \quad , \qquad \forall\, f = \begin{pmatrix} f^+ \\ f^- \end{pmatrix} \ . \tag{1.67}$$

For a proof of this fact, we just remark that, for any $f \in \mathcal{K}$, we have:

$$w\tau f = w_+(\tau f)_+ + w_-(\tau f)_- = w_+\tau f_- + w_-\tau f_+ = \tau w_- f_- + \tau w_+ f_+ = \tau w f \ , \tag{1.68}$$

proving $\tau w \tau = w$. The unitarity of $w$ also follows easily. The homogeneous Bogoliubov transformation $w$ we have thus constructed, maps the decomposition subspaces $\mathcal{K}_\pm$ and $\tilde{\mathcal{K}}_\pm$ onto each other. It is of course unique up to the choice of $w_+$, only.

### 1.1.4 Fermion Many-Particle Systems, CAR Algebra

Along the same lines as in Subsection 1.1.2, we now proceed to construct the fermion Fock space. To this end, we introduce the projection $\mathcal{S}_-$ onto the totally anti-symmetric subspace of $\mathcal{F}$ by setting

$$\mathcal{S}_- \psi_1 \otimes \cdots \otimes \psi_n := \frac{1}{n!} \sum_{\pi \in S_n} \operatorname{sign}(\pi)\, \psi_{\pi(1)} \otimes \cdots \otimes \psi_{\pi(n)} \quad , \qquad \forall\, \psi_1, \ldots, \psi_n \in \mathcal{H}^1 \ . \tag{1.69}$$

Just as in the boson case, this defines an orthogonal projection in $\mathcal{F}$ by linearity and by the fact that $\mathcal{S}_-$ is bounded on the finite vectors. We define the fermion Fock space, its subspace of finite vectors $F_-$ and its $n$-particle subspaces by:

$$\mathcal{F}_- := \mathcal{S}_- \mathcal{F} \ , \qquad F_- := \mathcal{S}_- F \ , \qquad \mathcal{H}^n_- := \mathcal{S}_- \mathcal{H}^n \ . \tag{1.70}$$

For any $f \in \mathcal{H}^1$, we introduce the fermion particle annihilation operators and fermion particle creation operators:

$$a(f) := \mathcal{S}_- a_\circ(f) \mathcal{S}_- \qquad \text{and} \qquad a^*(f) := \mathcal{S}_- a^*_\circ(f) \mathcal{S}_- \ . \tag{1.71}$$

Again, $F_-$ is an invariant subspace of these operators. (We shall later see that these operators extend to $\mathcal{F}_-$.) In contrast to the boson case they obey, for all $f, g \in \mathcal{H}^1$, the following canonical anti-commutation relations (CAR):

$$\{a(f), a^*(g)\} = \langle f \,|\, g \rangle \cdot \mathbf{1} \ , \qquad \{a(f), a(g)\} = \{a^*(f), a^*(g)\} = \mathbf{0} \ , \tag{1.72}$$

where $\{A, B\} := AB + BA$, for any two operators $A$ and $B$ in $\mathcal{F}_-$.

*Proof:* We prove relations (1.72) on finite vectors, only. We shall later see that they extend to the whole of $\mathcal{F}_-$. By linearity, it suffices to show the anti-commutation relations on elements of the form

$$\psi = \mathcal{S}_- \psi_1 \otimes \cdots \otimes \psi_n \ \in \ \mathcal{H}^n_- \ . \tag{1.73}$$

First, we remark that, for all such $\psi$ and all $f \in \mathcal{H}^1$, we have:

$$a^*(f) \mathcal{S}_- \psi_1 \otimes \cdots \otimes \psi_n = \sqrt{n+1} \cdot \mathcal{S}_- f \otimes \psi_1 \otimes \cdots \otimes \psi_n \ ,$$
$$a(f) \mathcal{S}_- \psi_1 \otimes \cdots \otimes \psi_n = \frac{1}{\sqrt{n!}} \sum_{j=1}^{n} (-1)^{j+1} \langle f \,|\, \psi_j \rangle\, \mathcal{S}_- \psi_1 \otimes \cdots \otimes \widehat{\psi_j} \otimes \cdot \otimes \psi_n \ .$$

Again, we indicate by $\widehat{\psi_j}$ that the corresponding factor is absent in the above tensor product. With the aid of these relations we obtain, for all $f, g \in \mathcal{H}^1$, on the one hand

$$\begin{aligned} a(f)a^*(g)\mathcal{S}_-\psi_1 \otimes \cdots \otimes \psi_n &= \sqrt{n+1} \cdot a(f)\mathcal{S}_- g \otimes \psi_1 \otimes \cdots \otimes \psi_n \\ &= \langle f \,|\, g \rangle \, \mathcal{S}_-\psi_1 \otimes \cdots \otimes \psi_n + \sum_{j=1}^{n} (-1)^j \, \langle f \,|\, \psi_j \rangle \, \mathcal{S}_- g \otimes \psi_1 \otimes \cdots \otimes \widehat{\psi_j} \otimes \cdots \otimes \psi_n \end{aligned} \tag{1.74}$$

and, on the other hand,

$$\begin{aligned} a^*(g)a(f)\mathcal{S}_-\psi_1 \otimes \cdots \otimes \psi_n &= \sqrt{n} \cdot \sum_{j=1}^{n} (-1)^{j+1} \, \langle f \,|\, \psi_j \rangle \, a^*(g)\mathcal{S}_-\psi_1 \otimes \cdots \otimes \widehat{\psi_j} \otimes \cdots \otimes \psi_n \\ &= - \sum_{j=1}^{n} (-1)^j \, \langle f \,|\, \psi_j \rangle \, \mathcal{S}_- g \otimes \psi_1 \otimes \cdots c \otimes \widehat{\psi_j} \otimes \cdots \otimes \psi_n \; . \end{aligned} \tag{1.75}$$

This proves the first of the three relations claimed. The second and the third of the relations are easily proved. □

In contrast to the fermion case, it turns out that the fermion particle annihilation and creation operators are in fact bounded operators. Namely, we have by the adjointness relation (1.24), for all normalized $\psi \in F_-$ and arbitrary $f \in \mathcal{H}^1$:

$$\| \, a(f)\psi \, \|^2 = \langle \psi \,|\, a^*(f)a(f)\psi \rangle = \big\langle \psi \,\big|\, \big(\mathbf{1} - a(f)a^*(f)\big)\psi \big\rangle = 1 - \| \, a^*(f)\psi \, \| \leq 1 \; . \tag{1.76}$$

An analogous estimate shows that $a^*(f)$ is also bounded. We shall from now on consider $a^*(f)$ and $a(f)$ as elements in $\mathcal{B}(\mathcal{F}_-)$, for all $f \in \mathcal{H}^1$. The algebra of polynomials in fermion particle creation an annihilation operators is thus a normed $*$-algebra, which by canonical completion gives rise to a $C^*$-algebra. This algebra is called the CAR Algebra. Also, the boundedness of $a(\cdot)$ and $a^*(\cdot)$ is the reason, why the anti-commutation relations (1.72) hold on the whole of $\mathcal{F}_-$. Furthermore, it follows from the adjointness relation (1.24) that

$$a^*(f) = \big(a(f)\big)^* \qquad \text{and} \qquad \big(a^*(f)\big)^* = a(f) \quad , \qquad \forall \; f \in \mathcal{H}^1. \tag{1.77}$$

### 1.1.5 The Self-Dual CAR Algebra

Quite analogously to the boson case, we now formulate the CAR Algebra in a self-dual fashion. In this case, however, the particle-hole space turns out to be itself a Hilbert space and is thus much easier to handle.

We consider the linear space $\mathcal{L}$ given by column vectors with two entries taken from $\mathcal{H}^1$, i. e.,

$$\mathcal{L} := \left\{ \begin{pmatrix} f^+ \\ f^- \end{pmatrix} \;\Big|\; f^\pm \in \mathcal{H}^1 \right\} \; , \tag{1.78}$$

where we agree to define the sum of two vectors and the exterior product in the standard way. For any $f \in \mathcal{L}$, we denote the first entry by $f^+$ and the second entry by $f^-$, thus defining the projections $f \mapsto f^\pm$ from $\mathcal{L}$ into $\mathcal{H}^1$. Together with the scalar product

$$\langle f \,|\, g \rangle_{\mathcal{L}} := \big\langle f^+ \,\big|\, g^+ \big\rangle_{\mathcal{H}^1} + \big\langle f^- \,\big|\, g^- \big\rangle_{\mathcal{H}^1} \quad , \qquad \forall \; f, g \in \mathcal{L} \; , \tag{1.79}$$

the space $\mathcal{L}$ is a Hilbert space. Whenever it is clear from the context which scalar product is meant, we shall drop the indices $\mathcal{L}$ and $\mathcal{H}^1$ from the symbols $\langle \cdot \,|\, \cdot \rangle$.

Obviously, $\mathcal{L}$ admits the decomposition into a direct orthogonal sum

$$\mathcal{L} = \mathcal{L}_+ \oplus \mathcal{L}_- \ , \qquad \mathcal{L}_+ := \left\{ \begin{pmatrix} f \\ 0 \end{pmatrix} \,\middle|\, f \in \mathcal{H}^1 \right\} , \qquad \mathcal{L}_- := \left\{ \begin{pmatrix} 0 \\ f \end{pmatrix} \,\middle|\, f \in \mathcal{H}^1 \right\} . \tag{1.80}$$

Let a conjugation $\tau : \mathcal{L} \to \mathcal{L}$ be defined as in Subsection 1.1.3 in terms of a conjugation $f \mapsto \bar{f}$ in $\mathcal{H}^1$, which is assumed to be compatible with the scalar product according to (1.55). Then $\tau$ acts on $\mathcal{L}$ by

$$\tau \begin{pmatrix} f^+ \\ f^- \end{pmatrix} := \begin{pmatrix} \bar{f}^- \\ \bar{f}^+ \end{pmatrix} \quad , \qquad \forall\, f \in \mathcal{L} \ . \tag{1.81}$$

The conjugation $\tau$ is itself compatible with the scalar product on $\mathcal{L}$, i. e., it has the property

$$\langle \tau f \,|\, \tau g \rangle = \overline{\langle f \,|\, g \rangle} = \langle g \,|\, f \rangle \quad , \qquad \forall\, f, g \in \mathcal{L} \ . \tag{1.82}$$

Any decomposition of $\mathcal{L}$ into an orthogonal direct sum of two subspaces $\mathcal{L} = \tilde{\mathcal{L}}_+ \oplus \tilde{\mathcal{L}}_-$ is called <u>self-dual</u>, if it satisfies

$$\tau \tilde{\mathcal{L}}_\pm = \tilde{\mathcal{L}}_\mp \ . \tag{1.83}$$

Note that it is implied that the two components of a self-dual decomposition are unitarily equivalent. Obviously, decomposition (1.80) is self-dual.

For any $f \in \mathcal{L}$, let us single out two elements of the CAR Algebra by defining:

$$B(f) := a^*(f^+) + a(\bar{f}^-) \ , \qquad B^*(f) := a^*(\bar{f}^-) + a(f^+) \ . \tag{1.84}$$

Obviously the algebra elements $B(f)$ and $B^*(f)$ are chosen to be adjoint to each other and we have

$$B^*(f) = \big(B(f)\big)^* = B(\tau f) \quad , \qquad \forall\, f \in \mathcal{L} \ . \tag{1.85}$$

The interpretation of the objects introduced in this subsection is completely analogous to the boson case.

The linear functionals $B(\cdot)$ allow us to treat the particle annihilation and particle creation operators on an equal footing. We can thus rewrite the CAR in the following condensed form:

$$\{B^*(f), B(g)\} = \langle f \,|\, g \rangle \cdot \mathbf{1} \quad , \qquad \forall\, f, g \in \mathcal{L} \ . \tag{1.86}$$

Even though the $C^*$-algebra obtained by taking the closure in the operator norm of the algebra generated by the operator-valued functional $B(\cdot)$ is no other algebra than the CAR Algebra, it is in this context common to term it the <u>self-dual CAR Algebra over $\mathcal{H}^1$</u>.

Again, there is a distinguished real subspace in $\mathcal{L}$, given by those elements which are real with respect to the conjugation $\tau$, namely

$$\mathcal{L}_{\mathbb{R}} := \{ f \in \mathcal{L} \mid \tau f = f \} = \left\{ \begin{pmatrix} f \\ \bar{f} \end{pmatrix} \,\middle|\, f \in \mathcal{H}^1 \right\} . \tag{1.87}$$

To each element in $\mathcal{L}_{\mathbb{R}}$ we may assign an element in $\mathcal{H}^1$ and vice-versa as in (1.63). Note again, that this correspondence is bijective but not an isomorphism, because it is not complex-linear.

According to the interpretation of $\mathcal{L}$ as particle-hole space, we may view homogeneous Bogoliubov transformations (see Chapter 2) of the CAR Algebra as unitary operators in $\mathcal{L}$ obeying the additional condition $\tau w \tau = w$. The unitarity of $w$ guarantees that the anti-commutation relations (1.86) are left invariant, while the second condition means that particles and holes are to be transformed in a manner dual to each other. Furthermore, it is clear that if $w$ is a homogeneous Bogoliubov transformation, then

$$\mathcal{L} = \tilde{\mathcal{L}}_+ \oplus \tilde{\mathcal{L}}_- \tag{1.88}$$

with $\tilde{\mathcal{L}}_\pm := w\mathcal{L}_\pm$, is again a self-dual decomposition. Conversely, if we are given a self-dual decomposition (1.88), then the subspaces $\tilde{\mathcal{L}}_\pm$ and $\mathcal{L}_\pm$ are unitarily equivalent. Now suppose $w_+ : \mathcal{L}_+ \to \tilde{\mathcal{L}}_+$ is a unitary mapping, then $w_- := \tau w_+ \tau$ is also unitary and

$$wf := w_+ f_+ + w_- f_- \quad , \qquad \forall\, f \in \mathcal{L} \tag{1.89}$$

defines a homogeneous Bogoliubov transformation $w$ mapping the components of the two decompositions onto each other. The notation $f_\pm$ is defined as in the boson case (see Subsection 1.1.3). Obviously $w$ is unique up to the choice of $w_+$, only.

## 1.2 States and Truncated Functionals

The fundamental object of quantum statistics is the algebra of observables. In the fermion case, this is a sub-algebra of the CAR Algebra, while in the boson case it is indirectly coded in the Weyl Algebra.

### 1.2.1 Bosonic States

We remind the reader that $\mathcal{W}\left(\mathcal{H}^1\right)$ is the closure of the algebra generated by the Weyl operators. It coincides with $\mathcal{B}(\mathcal{H}^1)$.

**Definition 1.7.** *A continuous*[2] *functional $\omega : \mathcal{W}\left(\mathcal{H}^1\right) \to \mathbb{C}$ is called a state, if it is positive and normalized, i. e., if*

$$\omega(w^* w) \geq 0 \qquad \textit{and} \qquad \omega(\mathbf{1}) = 1 \ , \tag{1.90}$$

*for all $w \in \mathcal{W}\left(\mathcal{H}^1\right)$.*

Another set of states is given by the so-called analytic states. They can be treated analogously to the states of the CAR Algebra.

[2] In fact, continuity is implied by positivity and the $C^*$-properties of the algebra. We could thus do without this additional assumption.

**Definition 1.8.** *A state $\omega$ on the Weyl Algebra is called an analytic state, if the mapping*

$$t \in \mathbb{R} \;\mapsto\; \omega\big(W(tf)\big) \tag{1.91}$$

*is analytic in an open strip around the real axis, for any $f \in \mathcal{H}^1$.*

As shown in [13], it suffices to demand analyticity in some neighborhood of zero, thus simplifying the above definition. This concept of analyticity is tailor-made to admit the following truncation of a state, which is central to HFB-Theory:

$$\omega^{(t)}\big(W(tf)\big) := \sum_{k=0}^{\infty} \frac{t^k}{k!} \frac{d^k}{ds^k} \log \omega\big(W(sf)\big)\Big|_{s=0} , \tag{1.92}$$

for any $t$ in a neighborhood $u_f \subseteq \mathbb{C}$ of zero. (Since $\omega$ is continuous, there always exists a neighborhood $u_f$, such that $\mathrm{Re}\,\omega\big(W(tf)\big) > \frac{1}{2}$, for all $t \in u_f$. This is all we need to make sense of the above definition.) Equivalently, we could define $\omega^{(t)}$ by demanding: In any finite dimensional subspace $V \subseteq \mathcal{H}^1$

$$\omega^{(t)}\big(W(f)\big) = \log \omega\big(W(f)\big) \tag{1.93}$$

holds, for all $f$ in some neighborhood $U \subseteq V$ of zero.

Analyticity of a state $\omega$ also allows us to define the expectation values of all polynomials of boson fields in that state in the following fashion:

$$\omega\big(\Phi(f_1)\cdots\Phi(f_n)\big) := (-i)^n \frac{d}{dt_1} \cdots \frac{d}{dt_n} \omega\big(W(t_1 f_1)\cdots W(t_n f_n)\big)\Big|_{t_1,\dots,t_n=0} . \tag{1.94}$$

The well-definedness and particularly the consistency with the commutation relations (1.37) follow from the concatenation rule (1.49) of Weyl operators. By linear extension to the complex plane, it is also possible to give meaning to expectation values of the form

$$\omega\big(a^{\tau_1}(f_1)\cdots a^{\tau_n}(f_n)\big) \quad , \qquad \forall\, \tau_1,\dots,\tau_n \in \{\varnothing, *\} \ , \ f_1,\dots,f_n \in \mathcal{H}^1 . \tag{1.95}$$

We now proceed to define the hierarchy of truncated functionals associated to any analytic state $\omega$. We define

$$\omega^{(t)}(f_1,\dots,f_n) := (-i)^n \frac{d}{dt_1} \cdots \frac{d}{dt_n} \log \omega\big(W(t_1 f_1)\cdots W(t_n f_n)\big)\Big|_{t_1,\dots,t_n=0} , \tag{1.96}$$

for any $f_1,\dots,f_n \in \mathcal{H}^1$. Note that we have, by (1.93) and (1.49):

$$\omega^{(t)}(\underbrace{f,\dots,f}_{n \text{ entries}}) = (-i)^n \frac{d^n}{dt^n} \omega^{(t)}\big(W(tf)\big)\Big|_{t=0} \quad , \qquad \forall\, f \in \mathcal{H}^1 . \tag{1.97}$$

The set of all functionals

$$f_1,\dots,f_n \;\mapsto \omega^{(t)}(f_1,\dots,f_n) \quad , \qquad \forall\, n \in \mathbb{N},\ f_1,\dots,f_n \in \mathcal{H}^1 , \tag{1.98}$$

linear in each entry, is called the hierarchy of truncated functionals associated to the state $\omega$. For any such hierarchy, we have, by (1.49), the commutation relation

$$\begin{aligned} \omega^{(t)}(f,g) - \omega^{(t)}(g,f) &= -\frac{d}{dt}\frac{d}{ds} \left( \log \frac{\omega\big(W(tf)W(sg)\big)}{\omega\big(W(sg)W(tf)\big)} \right) \Big|_{s=t=0} \\ &= -\frac{d}{dt}\frac{d}{ds}\big( - its \,\mathrm{Im}\, \langle f \,|\, g \rangle \,\big)\big|_{s=t=0} = i \,\mathrm{Im}\, \langle f \,|\, g \rangle \ , \end{aligned} \tag{1.99}$$

for all $f, g \in \mathcal{H}^1$.

The assumption of analyticity in Definition 1.8 entails that any analytic state $\omega$ is completely determined if we specify all the values of either

$$\omega\big(\Phi(f_1)\cdots\Phi(f_n)\big) \qquad \text{or} \qquad \omega^{(t)}(f_1,\dots,f_n) \ , \tag{1.100}$$

for all $n \in \mathbb{N}$ and all $f_1,\dots,f_n \in \mathcal{H}^1$.

In the next theorem we would like to see, how these two hierarchies of functionals are related to each other. Before doing so, we need to introduce the notion of the partition of a set. Let a finite set $M$ be given and denote by $P$ a set of nonempty, pairwise disjoint subsets $p^{(1)},\dots,p^{(k)}$ of $M$, called <u>cells</u>. We shall call $P$ a <u>partition of $M$</u> if

$$M = p^{(1)} \,\dot\cup\, \cdots \,\dot\cup\, p^{(k)} \ . \tag{1.101}$$

The elements of any $p$, itself an element of a partition $P$ of $M$, are denoted by $p_1, p_2, \dots$. All the partitions $P$ of $M$ together form a set denoted by $\mathcal{P}(M)$. If $M$ is of the form $M = \{1,\dots,n\}$, for a suitable $n$, we shall denote this set also by $\mathcal{P}_n$.

**Theorem 1.9.** *If a state $\omega$ is analytic, the hierarchy of truncated functionals $\omega^{(t)}$ satisfies*

$$\omega\big(\Phi(f_1)\cdots\Phi(f_n)\big) = \sum_{P\,\in\,\mathcal{P}_n}\prod_{p\in P}\omega^{(t)}(f_{p_1}, f_{p_2},\dots) \ , \tag{1.102}$$

*for all $f_1,\dots,f_n \in \mathcal{H}^1$. Here, we have additionally assumed that the mappings $j \mapsto p_j$ are strictly increasing for all cells $p$.*

Before we prove this theorem (see p. 27), let us remark that (1.102) is often used to *define* the hierarchy of truncated functionals. In particular, we can recursively solve (1.102) to find:

$$\begin{aligned}
\omega^{(t)}(f_1) &= \omega\big(\Phi(f_1)\big) \ ,\\
\omega^{(t)}(f_1,f_2) &= \omega\big(\Phi(f_1)\Phi(f_2)\big) - \omega\big(\Phi(f_1)\big)\omega\big(\Phi(f_2)\big) \ ,\\
\omega^{(t)}(f_1,f_2,f_3) &= \omega\big(\Phi(f_1)\Phi(f_2)\Phi(f_3)\big) - \omega\big(\Phi(f_1)\big)\omega\big(\Phi(f_2)\Phi(f_3)\big)\\
&\quad - \omega\big(\Phi(f_2)\big)\omega\big(\Phi(f_1)\Phi(f_3)\big) - \omega\big(\Phi(f_3)\big)\omega\big(\Phi(f_1)\Phi(f_2)\big)\\
&\quad + 2\omega\big(\Phi(f_1)\big)\omega\big(\Phi(f_2)\big)\omega\big(\Phi(f_3)\big)
\end{aligned}$$

and

$$\begin{aligned}
\omega^{(t)}(f_1,f_2,f_3,f_4) &= \omega\big(\Phi(f_1)\Phi(f_2)\Phi(f_3)\Phi(f_4)\big) - \omega\big(\Phi(f_1)\big)\omega\big(\Phi(f_2)\Phi(f_3)\Phi(f_4)\big)\\
&\quad - \omega\big(\Phi(f_2)\big)\omega\big(\Phi(f_1)\Phi(f_3)\Phi(f_4)\big) - \omega\big(\Phi(f_3)\big)\omega\big(\Phi(f_1)\Phi(f_2)\Phi(f_4)\big)\\
&\quad - \omega\big(\Phi(f_4)\big)\omega\big(\Phi(f_1)\Phi(f_2)\Phi(f_3)\big) - \omega\big(\Phi(f_1)\Phi(f_2)\big)\omega\big(\Phi(f_3)\Phi(f_4)\big)\\
&\quad - \omega\big(\Phi(f_1)\Phi(f_3)\big)\omega\big(\Phi(f_2)\Phi(f_4)\big) - \omega\big(\Phi(f_1)\Phi(f_4)\big)\omega\big(\Phi(f_2)\Phi(f_3)\big)\\
&\quad + 2\omega\big(\Phi(f_1)\big)\omega\big(\Phi(f_2)\big)\omega\big(\Phi(f_3)\Phi(f_4)\big) + 2\omega\big(\Phi(f_1)\big)\omega\big(\Phi(f_3)\big)\omega\big(\Phi(f_2)\Phi(f_4)\big)\\
&\quad + 2\omega\big(\Phi(f_1)\big)\omega\big(\Phi(f_4)\big)\omega\big(\Phi(f_2)\Phi(f_3)\big) + 2\omega\big(\Phi(f_2)\big)\omega\big(\Phi(f_3)\big)\omega\big(\Phi(f_1)\Phi(f_4)\big)\\
&\quad + 2\omega\big(\Phi(f_2)\big)\omega\big(\Phi(f_4)\big)\omega\big(\Phi(f_1)\Phi(f_3)\big) + 2\omega\big(\Phi(f_3)\big)\omega\big(\Phi(f_4)\big)\omega\big(\Phi(f_1)\Phi(f_2)\big)\\
&\quad - 6\omega\big(\Phi(f_1)\big)\omega\big(\Phi(f_2)\big)\omega\big(\Phi(f_3)\big)\omega\big(\Phi(f_4)\big) \ .
\end{aligned} \tag{1.103}$$

The proof of Theorem 1.9 is based on two lemmas. The first lemma clarifies, how we obtain from the partitions of the set of the first $n$ positive integers, the partitions of the set of the first $n+1$ positive integers. We consider the proof of this lemma to be trivial.

**Lemma 1.10.** *Let $n$ be a positive integer. We then have:*

$$\mathcal{P}_{n+1} = \bigcup_{\{p^{(1)},p^{(2)},\dots\}\in\mathcal{P}_n} \quad \bigcup_{j=0,1,2,\dots} \left\{\left\{p^{(1)},\dots,p^{(j)} \cup \{n+1\}, p^{(j+1)},\dots\right\}\right\} \tag{1.104}$$

*For $j=0$ we agree that the set on very right hand side equals $\{\{n+1\}, p^{(1)}, p^{(2)}, \dots\}$.*

The second lemma is essentially the proof of Theorem 1.9. We formulate it as a lemma in order to clarify the mathematical structure behind the theorem.

**Lemma 1.11.** *For any positive integer $n$ and any function $f : \mathbb{R}^n \to \mathbb{C}$, at least $n$ times continuously differentiable in a neighborhood $U$ of zero, the following is true:*

$$\frac{d}{dt_n}\cdots\frac{d}{dt_1} e^{f(t_1,\dots,t_n)} = e^{f(t_1,\dots,t_n)} \cdot \sum_{P\in\mathcal{P}_n}\prod_{p\in P}\left(\frac{d}{dt_{p_1}}\frac{d}{dt_{p_2}}\cdots f(t_1,\dots,t_n)\right) , \tag{1.105}$$

*for all $(t_1,\dots,t_n) \in U$.*

*Proof:* We give an induction argument. The claim is trivial in the case $n=1$. Now suppose the claim was true for an arbitrary $n \in \mathbb{N}$. Then it is also true that

$$\begin{aligned}\frac{d}{dt_{n+1}}\cdots\frac{d}{dt_1} e^{f(t_1,\dots,f_{n+1})} &= \frac{d}{dt_{n+1}} e^{f(t_1,\dots,t_{n+1})} \cdot \sum_{P\in\mathcal{P}_n}\prod_{p\in P}\left(\frac{d}{dt_{p_1}}\frac{d}{dt_{p_2}}\cdots f(t_1,\dots,t_{n+1})\right)\\ &= e^{f(t_1,\dots,t_{n+1})}\left[\frac{d}{dt_{n+1}} f(t_1,\dots,t_{n+1})\right]\sum_{P\in\mathcal{P}_n}\prod_{p\in P}\left(\frac{d}{dt_{p_1}}\frac{d}{dt_{p_2}}\cdots f(t_1,\dots,t_{n+1})\right)\\ &\quad + e^{f(t_1,\dots,t_{n+1})}\frac{d}{dt_{n+1}}\sum_{P\in\mathcal{P}_n}\prod_{p\in P}\left(\frac{d}{dt_{p_1}}\frac{d}{dt_{p_2}}\cdots f(t_1,\dots,t_{n+1})\right) .\end{aligned}$$

Leibniz' rule together with Lemma 1.10 (the first term in the sum on the right hand side corresponds to $j=0$) allows us to deduce from this

$$\frac{d}{dt_{n+1}}\cdots\frac{d}{dt_1} e^{f(t_1,\dots,t_{n+1})} = e^{f(t_1,\dots,t_{n+1})} \cdot \sum_{P\in\mathcal{P}_{n+1}}\prod_{p\in P}\left(\frac{d}{dt_{p_1}}\frac{d}{dt_{p_2}}\cdots f(t_1,\dots,t_{n+1})\right) . \tag{1.106}$$

□

*Proof of Theorem 1.9:* Let us first note that, due to the concatenation relation (1.49),

$$W(f_1)\cdots W(f_n) = e^{s(f_1,\dots,f_n)} W(f_1+\cdots+f_n) , \tag{1.107}$$

with

$$s(f_1,\dots,f_n) := \frac{i}{2}\sum_{k<k'} \operatorname{Im}\langle f_k \mid f_{k'}\rangle , \tag{1.108}$$

is true for all $f_1, \dots, f_n \in \mathcal{H}^1$. Thus we obtain from (1.93):

$$\begin{aligned}\omega\big(W(f_1)\cdots W(f_n)\big) &= e^{s(f_1,\dots,f_n)} e^{\omega^{(t)}\left(W(f_1+\dots+f_n)\right)} \\ &= \exp\left(e^{-s(f_1,\dots,f_n)}\omega^{(t)}\big(W(f_1)\cdots W(f_n)\big) + s(f_1,\dots,f_n)\right) \ . \qquad (1.109)\end{aligned}$$

We therefore have by Lemma 1.11:

$$\begin{aligned}\omega\big(\Phi(f_1)\cdots\Phi(f_n)\big) &= \frac{d}{dt_1}\cdots\frac{d}{dt_n}\exp\bigg(e^{-s(t_1f_1,\dots,t_nf_n)}\omega^{(t)}\big(W(t_1f_1)\cdots W(t_nf_n)\big) \\ &\qquad + s(t_1f_1,\dots,t_nf_n)\bigg)\bigg|_{t_1=\dots=t_n=0} \\ &= \sum_{P\in\mathcal{P}_n}\prod_{p\in P}\left(\frac{d}{dt_{p_1}}\frac{d}{dt_{p_2}}\cdots\Big\{e^{-s(t_{p_1}f_{p_1},t_{p_2}f_{p_2},\dots)}\omega^{(t)}\big(W(t_{p_1}f_{p_1})W(t_{p_2}f_{p_2})\cdots\big)\right. \\ &\qquad \left. + s(t_{p_1}f_{p_1},t_{p_2}f_{p_2},\dots)\Big\}\Big|_{t_{p_1}=t_{p_2}=\dots=0}\right) \\ &= \sum_{P\in\mathcal{P}_n}\prod_{p\in P}\left(\frac{d}{dt_{p_1}}\frac{d}{dt_{p_2}}\cdots\log\left\{\omega\big(W(t_{p_1}f_{p_1})W(t_{p_2}f_{p_2})\cdots\big)\right\}\Big|_{t_{p_1}=t_{p_2}=\dots=0}\right) \\ &= \sum_{P\in\mathcal{P}_n}\prod_{p\in P}\omega^{(t)}(f_{p_1},f_{p_2},\dots) \ . \qquad (1.110)\end{aligned}$$

This proves the claim. □

### 1.2.2 Fermionic States

**Definition 1.12.** *A continuous functional $\omega : \mathcal{A}_{car}(\mathcal{H}^1) \to \mathbb{C}$ is called a state, if it is positive and normalized, i. e., if it satisfies*

$$\omega(a^*a) \geq 0 \qquad \text{and} \qquad \omega(\mathbf{1}) = 1 \ , \qquad (1.111)$$

*for all $a \in \mathcal{A}_{car}(\mathcal{H}^1)$.*

By the fact that the CAR Algebra is itself a $C^*$-algebra, the states can be directly defined as functionals on this algebra, and we may define the properties we are interested in directly in terms of the particle annihilation and particle creation operators. However, before introducing the concept of the hierarchy of truncated functionals, we have yet to define the sign of a partition. To this end, let $M = \{m_1; m_2; \dots\}$ be an ordered set with finitely many elements (in order to emphasize that we want to keep track of the order of the elements of $M$, we shall always enumerate them with semicolons) and let $P$ be a partition of $M$ in the sense we specified in Subsection 1.2.1. Let us now denote the cells of $P$ by $p^{(1)}, \dots, p^{(k)}$, such that

$$j < j' \qquad \Rightarrow \qquad \min\left(p^{(j)}\right) < \min\left(p^{(j')}\right) \quad , \qquad \forall\ j, j' \qquad (1.112)$$

and turn them into ordered sets

$$p^{(1)} = \{p_1^{(1)}; p_2^{(1)}; \dots\} \ , \quad \dots \quad , \quad p^{(k)} = \{p_1^{(k)}; p_2^{(k)}; \dots\} \qquad (1.113)$$

by adopting the order specified by the superset $M$. For a partition $P$, we define its sign, denoted by sign$(P)$, to be the sign of the permutation $\pi$ given by

$$\{m_{\pi(1)}; m_{\pi(2)}; \dots\} = \left\{\, p_1^{(1)}; p_2^{(1)}; \dots; p_1^{(2)}; p_2^{(2)}; \dots \;\; \dots; p_1^{(k)}; p_2^{(k)}; \dots \,\right\} , \tag{1.114}$$

where, obviously, equality is understood in the sense of ordered sets.

Without significant loss of generality, we may restrict the following considerations to so called <u>even states</u>, i. e., to states $\omega$ with the property

$$\omega\big(B(f_1)\cdots B(f_{2n-1})\big) = 0 \quad , \qquad \forall\; f_1, \dots, f_{2n-1} \in \mathcal{L},\; n \in \mathbb{N}\; . \tag{1.115}$$

For any such state, there is always one and only one <u>hierarchy $\omega^{(t)}$ of truncated functionals</u> determined by

$$\omega\big(B(f_1)\cdots B(f_n)\big) = \sum_{P \in \mathcal{P}_n} \operatorname{sign}(P) \prod_{p \in P} \omega^{(t)}(f_{p_1}, f_{p_2}, \dots)\; , \tag{1.116}$$

see [13]. We have again denoted the elements of any cell $p$ of $P$ by $p_1, p_2, \dots$ and assumed that the mappings $j \mapsto p_j$ are strictly increasing. Obviously the hierarchy of truncated functionals contains all information on $\omega$ there is. (Note that the ordering introduced in (1.112) of the cells of a partition $P$ is irrelevant for (1.116), by the assumption that $\omega$ is even.)

# Chapter 2

# Bogoliubov Transforms

## 2.1 Bosonic Theory

In this section $\mathcal{K}$ denotes the Krein space introduced in Subsection 1.1.3. For the definition of this concept and related notions, we refer the reader to Appendix A.

A bosonic Bogoliubov transformation is a pair $(w, v)$ of a bijective transformation

$$w : \mathcal{K} \to \mathcal{K} \ , \quad \text{such that} \qquad [wf \,|\, wg] = [f \,|\, g] \quad , \qquad \forall \ f, g \in \mathcal{K} \ , \tag{2.1}$$

additionally obeying $\tau w \tau = w$, and a linear functional $v$ on $\mathcal{K}$, additionally obeying $v(\tau \cdot) = \overline{v(\cdot)}$. If this functional vanishes identically, we say the above pair is a homogeneous Bogoliubov transformation, also denoted just by $w$. Otherwise we say the above pair is an inhomogeneous Bogoliubov transformation.

The properties of isometry with respect to the inner product and bijectivity of $w$ together, are called unitarity in the Krein space sense. It is equivalent to demand

$$w\, w^{[*]} = w^{[*]}\, w = \mathbf{1} \ , \tag{2.2}$$

where $w^{[*]}$ denotes the adjoint of $w$ with respect to the inner product $[\cdot \,|\, \cdot]$, defined in Appendix A. In that appendix we also introduce a norm on $\mathcal{K}$ and Theorem A.4 shows that any unitary operator in $\mathcal{K}$ is bounded.

To any Bogoliubov transformation $(w, v)$ we associate an algebra automorphism $\alpha_{(w,v)}$ of the Weyl Algebra given by

$$\alpha_{(w,v)}\Big(W\big(\rho^{-1}(f)\big)\Big) := e^{iv(f)} \cdot W\big(\rho^{-1}(wf)\big) \quad , \qquad \forall \ f \in \mathcal{K}_{\mathbb{R}} \ . \tag{2.3}$$

We recall the definition of the map $\rho$ given in (1.63) and the definition of $\mathcal{K}_{\mathbb{R}}$ given in (1.62). Due to the condition $\tau w \tau = w$, we have $f \in \mathcal{K}_{\mathbb{R}} \Rightarrow wf \in \mathcal{K}_{\mathbb{R}}$. The inverse Bogoliubov transformation

$$(w, v)^{-1} := \Big(w^{[*]}, -v\big(w^{[*]}(\cdot)\big)\Big) \tag{2.4}$$

is defined in such a way, as to ensure that $\alpha_{(w,v)} \circ \alpha_{(w,v)^{-1}}$ is the identity on the Weyl Algebra. We observe that the concatenation relations (1.49) are invariant under the action of the automorphism $\alpha$. To see this, we note

$$\operatorname{Im}\big\langle \rho^{-1}(f)\,\big|\,\rho^{-1}(g)\big\rangle_{\mathcal{H}^1} = \frac{1}{2}\,[f\,|\,g] \quad , \qquad \forall\ f,g \in \mathcal{K}_{\mathbb{R}}\ . \tag{2.5}$$

As an operator in $\mathcal{K}$, we may write the homogeneous part $w$ of a Bogoliubov transformation as a $2\times 2$ block matrix, with respect to the decomposition $\mathcal{K} = \mathcal{K}_+ {}^{[+]} \mathcal{K}_-$ introduced in Subsection 1.1.3, as follows:

$$w = \begin{pmatrix} X & Y \\ \bar{Y} & \bar{X} \end{pmatrix} \qquad \text{and} \qquad w^{[*]} = w^{-1} = \begin{pmatrix} X^* & -Y^T \\ -Y^* & X^T \end{pmatrix} , \tag{2.6}$$

for some $X, Y \in \mathcal{B}(\mathcal{H}^1)$. (For the second relation, see (A.20).) The unitarity condition (2.2) may equivalently be rewritten in terms of $X$ and $Y$:

$$XX^* - YY^* = \mathbf{1}\ , \qquad XY^T - YX^T = \mathbf{0}\ , \tag{2.7a}$$

$$X^*X - Y^T\bar{Y} = \mathbf{1}\ , \qquad X^*Y - Y^T\bar{X} = \mathbf{0}\ . \tag{2.7b}$$

An important point in this context is the question, whether or not there exists a unitary transformation $U$ of the boson Fock space $\mathcal{F}_+$ with the property

$$\alpha\big(W(f)\big) = UW(f)U^* \quad , \qquad \forall\ f \in \mathcal{H}^1\ . \tag{2.8}$$

If the answer is affirmative, we say that $(w, v)$ possesses a unitary implementation $U$. The central theorem in this context is:

**Theorem 2.1 (Shale-Steinspring).** *A Bogoliubov transformation $(w, v)$ possesses a unitary implementation, if and only if the operator $Y \in \mathcal{B}(\mathcal{H}^1)$ defined by (2.6) is Hilbert-Schmidt and $v : \mathcal{K} \to \mathbb{C}$ is continuous.*

## 2.2 Fermionic Theory

In this section $\mathcal{L}$ denotes the Hilbert space introduced in Subsection 1.1.5.

A (homogeneous) fermionic Bogoliubov transformation is a unitary transformation $w$ of the Hilbert space $\mathcal{L}$, obeying additionally $\tau w \tau = w$.

To any Bogoliubov transformation $w$ we associate an algebra automorphism, given by

$$\alpha_w\big(B(f)\big) := B(wf) \quad , \qquad \forall\ f \in \mathcal{L}\ , \tag{2.9}$$

where we use the self-dual notation introduced in Subsection 1.2.1. Equivalently, this relation may be expressed in terms of the fermion particle annihilation and creation operators, namely

$$\alpha_w\big(a(f)\big) \;=\; a(Xf) + a^*(Y\bar{f})\ . \tag{2.10}$$

Here the operators $X$ and $Y$, both in $\mathcal{B}(\mathcal{H}^1)$, are given by the following decomposition of $w$ in terms of the self-dual decomposition (1.80) of $\mathcal{L}$

$$w = \begin{pmatrix} X & Y \\ \bar{Y} & \bar{X} \end{pmatrix} \qquad \text{and} \qquad w^* = \begin{pmatrix} X^* & Y^T \\ Y^* & X^T \end{pmatrix} . \tag{2.11}$$

The unitarity of $w$ may be reexpressed in terms of $X$ and $Y$ in the following way:

$$XX^* + YY^* = \mathbf{1} \ , \qquad XY^T + YX^T = \mathbf{0} \ , \tag{2.12a}$$

$$X^*X + Y^T\bar{Y} = \mathbf{1} \ , \qquad X^*Y + Y^T\bar{X} = \mathbf{0} \ . \tag{2.12b}$$

An important point in this context is the question, whether or not there exists a unitary transformation $U$ of the fermion Fock space $\mathcal{F}_-$ such that

$$\alpha_{(w,v)}\big(B(f)\big) = UB(f)U^* \quad , \qquad \forall\ f \in \mathcal{L} \ . \tag{2.13}$$

If the answer is affirmative, we say that the Bogoliubov transformation $w$ possesses a unitary implementation $U$. The central theorem in this context is almost the same as in the boson case:

**Theorem 2.2 (Shale-Steinspring).** *A Bogoliubov transformation $w$ possesses a unitary implementation, if and only if the operator $Y \in \mathcal{B}(\mathcal{H}^1)$ defined by* (2.11) *is Hilbert-Schmidt.*

# Chapter 3

# Quasi-Free States and Generalized Density Matrices

We are now in the position to formulate what we mean by a quasi-free state. It is this set of states, which plays the central role in HFB-Theory.

## 3.1 Bosonic Theory

### 3.1.1 Quasi-Free States

In the bosonic theory we define the property of a state being quasi-free on the Weyl Algebra. We first give a definition, which is seemingly very restrictive. However, we shall see *a posteriori* that these states are more general than one might have expected.

**Definition 3.1.** *An analytic state $\omega$ is called a quasi-free state, if it satisfies, together with its truncated hierarchy $\omega^{(t)}$:*

$$\omega\big(W(f)\big) = e^{i\omega^{(t)}(f) - \frac{1}{2}\omega^{(t)}(f,f)} \quad , \qquad \forall\ f \in \mathcal{H}^1 \ . \tag{3.1}$$

Alternatively, the property of being quasi-free, may also be defined directly in terms of the truncated hierarchy of functionals, as follows.

**Theorem 3.2.** *An analytic state $\omega$ is quasi-free if and only if*

$$\omega^{(t)}(f_1, \ldots, f_n) = 0 \quad , \qquad \forall\ n \geq 3,\ f_1, \ldots, f_n \in \mathcal{H}^1 \ . \tag{3.2}$$

*Proof:* In view of the definition of quasi-freeness and of (1.96), the necessity of condition (3.2) is clear. It remains to prove its sufficiency. By construction, the mapping $t \in \mathbb{R} \mapsto \omega^{(t)}\big(W(tf)\big)$ is real analytic in a neighborhood of zero, for any $f \in \mathcal{H}^1$. By relation (1.97), we therefore have

$$\begin{aligned}\omega^{(t)}(W(tf)) &= \sum_{k=0}^{\infty} \frac{t^k}{k!} \frac{d^k}{ds^k} \omega^{(t)}(W(sf))|_{s=0} \\ &= \sum_{k=1}^{\infty} \frac{t^k}{k!} i^k \omega^{(t)}(\underbrace{f, \ldots, f}_{k \text{ entries}}) = it \cdot \omega^{(t)}(f) - \tfrac{1}{2} t^2 \omega^{(t)}(f, f) \ ,\end{aligned} \tag{3.3}$$

for any $f \in \mathcal{H}^1$. This fact, together with (1.93) proves that $\omega$ is quasi-free[1]. □

One feature of quasi-free states is that all expectation values in monomials of fields may be expressed in terms of expectation values of one and two fields. In particular, (3.2) together (1.102) yields

$$\begin{aligned}\omega\big(\Phi(f_1) \cdots \Phi(f_4)\big) &= \omega\big(\Phi(f_1)\Phi(f_2)\big)\omega\big(\Phi(f_3)\Phi(f_4)\big) \\ &\quad + \omega\big(\Phi(f_1)\Phi(f_3)\big)\omega\big(\Phi(f_2)\Phi(f_4)\big) + \omega\big(\Phi(f_1)\Phi(f_4)\big)\omega\big(\Phi(f_2)\Phi(f_3)\big) \\ &\quad - 2\omega\big(\Phi(f_1)\big)\omega\big(\Phi(f_2)\big)\omega\big(\Phi(f_3)\big)\omega\big(\Phi(f_4)\big) \ ,\end{aligned} \tag{3.4}$$

for all $f_1, \ldots, f_4 \in \mathcal{H}^1$.

We now show, following an idea of Robinson [29] (see also Baumann and Hegerfeldt [9]), that the set of quasi-free states is more general than one might have guessed from Definition 3.1 or Theorem 3.2. They are in fact the only states with a finite hierarchy of truncated functionals. The key element of this proof is a remarkable theorem in probability theory, known as Marcinkiewicz' Theorem. (See Theorem 3.6, below.)

**Theorem 3.3.** *If $\omega$ is an analytic state with the additional property that*

$$\omega^{(t)}(f_1, \ldots, f_n) = 0 \quad , \qquad \forall\, n \geq n_0,\ f_1, \ldots, f_n \in \mathcal{H}^1 \ , \tag{3.5}$$

*for some $n_0 \in \mathbb{N}$, then $\omega$ is quasi-free.*

Before proceeding to the proof of this theorem (see p. 39) we formulate the following lemma.

**Lemma 3.4.** *For any analytic state $\omega$, any $n \geq 3$ and arbitrary $f_1, \ldots, f_n \in \mathcal{H}^1$, we have:*

$$\omega^{(t)}\big(f_{\pi(1)}, \ldots, f_{\pi(n)}\big) = \omega^{(t)}(f_1, \ldots, f_n) \quad , \qquad \forall\, \pi \in S_n \ . \tag{3.6}$$

[1]Note that we use

$$\omega(W(f)) = \exp\big(\omega^{(t)}(W(f))\big) \quad , \qquad \forall\, f \in \mathcal{H}^1 \ . \tag{\#}$$

In particular we have not assumed that $f$ is small. Compare this to (1.93). Strictly speaking this implies that, for any fixed $f \in \mathcal{H}^1$, the mapping

$$t \ \mapsto \ \omega^{(t)}(W(tf)) := \log \omega\,(W(tf))$$

is understood as a multi-valued mapping in $\mathbb{C}$. This ambivalence is, however, irrelevant for (#).

*Proof:* Let $\omega$ be any analytic state and $f_1, f_2, f_3 \in \mathcal{H}^1$ arbitrary. Explicitly solving equations (1.102) in the cases $n = 1, 2, 3$ yields:

$$\begin{aligned}\omega^{(t)}(f_1, f_2, f_3) = \omega\big(\Phi(f_1)\Phi(f_2)\Phi(f_3)\big) \\ - \omega\big(\Phi(f_1)\Phi(f_2)\big)\omega\big(\Phi(f_3)\big) - \omega\big(\Phi(f_1)\Phi(f_3)\big)\omega\big(\Phi(f_2)\big) \\ - \omega\big(\Phi(f_2)\Phi(f_3)\big)\omega\big(\Phi(f_1)\big) + 2\omega\big(\Phi(f_1)\big)\omega\big(\Phi(f_2)\big)\omega\big(\Phi(f_3)\big) \ . \quad (3.7)\end{aligned}$$

With the aid of this identity, the commutation relations (1.37) and with linearity, it is easy to see that the statement of the lemma is true for $n = 3$. To prove (3.6) for $n > 3$ it is clearly sufficient to show that, given arbitrary $f_1, \ldots, f_n \in \mathcal{H}^1$,

$$\omega^{(t)}\left(f_{\pi(1)}, \ldots, f_{\pi(n)}\right) = \omega^{(t)}(f_1, \ldots, f_n) \quad (3.8)$$

holds, for any transposition $\pi \in S_n$ of the type

$$\pi(1) = 1, \ \ldots, \ \pi(i) = i + 1, \ \pi(i + 1) = i, \ \ldots, \ \pi(n) = n \ . \quad (3.9)$$

We show this by an induction argument. Let $n > 3$ be given and suppose the statement of the lemma to be true, for all $n' < n$. Then we have by Theorem 1.9

$$\begin{aligned}&\omega^{(t)}\left(f_{\pi(1)}, \ldots, f_{\pi(n)}\right) \\ &= \underbrace{\omega\left(\Phi(f_{\pi(1)}) \cdots \Phi(f_{\pi(n)})\right)}_{=:\ \text{term } 1} - \overbrace{\sum_{P \in \mathcal{P}_n \setminus \{\{1,\ldots,n\}\}} \prod_{p \in P} \omega^{(t)}\left(f_{\pi(p_1)}, f_{\pi(p_2)}, \ldots\right)}^{=:\ \text{term } 2} \ . \quad (3.10)\end{aligned}$$

The commutation relations (1.37) imply:

$$\text{term } 1 = \omega\big(\Phi(f_1) \cdots \Phi(f_n)\big) + i \, \mathrm{Im} \, \langle f_{i+1} \mid f_i \rangle \cdot \omega\left(\Phi(f_1) \cdots \widehat{\Phi(f_i)}\widehat{\Phi(f_{i+1})} \cdots \Phi(f_n)\right) \ , \quad (3.11)$$

where the notation $\widehat{\Phi(f_i)}$ and $\widehat{\Phi(f_{i+1})}$ indicates that these factors are absent in the above product. In the sum in term 2, we divide the set of partitions into three disjoint subsets $\mathcal{P}_n^1$, $\mathcal{P}_n^2$ and $\mathcal{P}_n^3$, such that

$$\mathcal{P}_n \ = \ \mathcal{P}_n^1 \ \dot\cup \ \mathcal{P}_n^2 \ \dot\cup \ \mathcal{P}_n^3 \ , \quad (3.12)$$

with:

1. Denote by $\mathcal{P}_n^1$ the set of all partitions in $\mathcal{P}_n \setminus \{\{1, \ldots, n\}\}$, containing the set $\{i, i+1\}$ as one cell.
2. Denote by $\mathcal{P}_n^2$ the set of all partitions in $\mathcal{P}_n \setminus \{\{1, \ldots, n\}\}$, where $\{i, i + 1\}$ appears as a subset of a cell containing at least three elements.
3. Denote by $\mathcal{P}_n^3$ the set of all partitions in $\mathcal{P}_n \setminus \{\{1, \ldots, n\}\}$, where $i$ and $i + 1$ are elements of different cells.

We then have:

$$\text{term } 2 \ = \ \text{term } 2.1 \ + \ \text{term } 2.2 \ + \ \text{term } 2.3 \ , \quad (3.13)$$

where

$$\text{term 2.j} := \sum_{P\in\mathcal{P}_n^j} \prod_{p\in P} \omega^{(t)}\big(f_{\pi(p_1)}, f_{\pi(p_2)}, \cdots\big) \quad , \qquad \forall\, j\in\{1,2,3\}\ . \tag{3.14}$$

We now consider these three expressions separately. For term 2.1 we have, by the commutation relations (1.99):

$$\begin{aligned}\text{term 2.1} &= \big\{\omega^{(t)}(f_i, f_{i+1}) + i\,\mathrm{Im}\,\langle f_{i+1}\,|\,f_i\rangle\big\} \sum_{P\in\mathcal{P}_n^1} \prod_{p\in P\setminus\{\{i,i+1\}\}} \omega^{(t)}\big(f_{\pi(p_1)}, f_{\pi(p_2)}, \dots\big)\\ &= \sum_{P\in\mathcal{P}_n^1} \prod_{p\in P} \omega^{(t)}(f_{p_1}, f_{p_2}, \dots) + i\,\mathrm{Im}\,\langle f_{i+1}\,|\,f_i\rangle\, \omega\Big(\Phi(f_1)\cdots\widehat{\Phi(f_i)}\widehat{\Phi(f_{i+1})}\cdots\Phi(f_n)\Big)\ .\end{aligned} \tag{3.15}$$

term 2.2 has the property that $f_i$ and $f_{i+1}$ always appear together in one cell of three or more, but less than $n$ elements, i. e., each summand in term 2.2 contains a factor of the form

$$\omega^{(t)}(f_k, \dots, f_{i+1}, f_i, \dots, f_{k+l})\ , \tag{3.16}$$

for some $k, l \in \{1, \dots, n-1\}$ with $l > 2$. By the induction hypothesis we have

$$(3.16) = \omega^{(t)}(f_k, \dots, f_i, f_{i+1}, \dots, f_{k+l}) \tag{3.17}$$

and therefore

$$\text{term 2.2} = \sum_{P\in\mathcal{P}_n^2} \prod_{p\in P} \omega^{(t)}(f_{p_1}, f_{p_2}, \dots)\ . \tag{3.18}$$

Finally, term 2.3 has the property that $f_i$ and $f_{i+1}$ appear always in different cells. Therefore, exchanging these elements corresponds to changing the order of summation over the elements of $\mathcal{P}_n^3$. Again, we obtain

$$\text{term 2.3} = \sum_{P\in\mathcal{P}_n^3} \prod_{p\in P} \omega^{(t)}(f_{p_1}, f_{p_2}, \dots)\ . \tag{3.19}$$

Inserting the expressions we obtained for term 1 and term 2 and using the cancellation between term 1 and term 2.1, we arrive at

$$\begin{aligned}\omega^{(t)}(f_{\pi(1)}, \dots, f_{\pi(n)}) &= \omega\big(\Phi(f_1)\cdots\Phi(f_n)\big) - \sum_{P\in\mathcal{P}_n\setminus\{\{1,\dots,n\}\}} \prod_{p\in P} \omega^{(t)}(f_{p_1}, f_{p_2})\\ &= \omega^{(t)}(f_1, \dots, f_n)\ .\end{aligned} \tag{3.20}$$

This completes the proof. □

We remark that by positivity and by analyticity of the state $\omega$, the map $t \mapsto \omega\big(W(tf)\big)$ on $\mathbb{R}$ is a function of positive type (see, e. g., [27]).

**Definition 3.5.** *A complex-valued, bounded, continuous function $f$ on $\mathbb{R}$ that has the property that $\big(f(t_i - t_j)\big)_{i,j}$ is a positive matrix on $\mathbb{C}^N$, for each $N$ and all $t_1, \dots, t_N \in \mathbb{R}$, is called a function of positive type.*

By Bochner's Theorem (see, e. g., Theorem IX.9 in [27]) and by the fact that $\omega$ is normalized, it follows that, for any $f \in \mathcal{H}^1$, there exists a probability measure $\mu_{\omega,f}$ such that:

$$\omega\big(W(tf)\big) = \int d\mu_{\omega,f}(a)e^{ita} \quad , \qquad \forall\, t \in \mathbb{R} \ . \tag{3.21}$$

Hence the mapping $t \mapsto \omega\big(W(tf)\big)$ is a characteristic function in the sense of probability theory. The following remarkable theorem (see e. g. [28]) holds.

**Theorem 3.6 (Marcinkiewicz).** *Let $\varphi$ be a characteristic function on $\mathbb{R}$ and $p$ be a polynomial such that*

$$\varphi(t) = e^{p(t)} \quad , \qquad \forall\, t \in \mathbb{R} \ . \tag{3.22}$$

*Then $p$ is of the form $p(t) = iat - bt^2$, for some $a \in \mathbb{R}$ and some $b \in \mathbb{R}_0^+$.*

*Proof of Theorem 3.3:* Due to the assumption that the truncated functionals of $\omega$ vanish for all orders higher than $n_0$, we have

$$\omega^{(t)}\big(W(f)\big) = \omega^{(t)}\big(W(tf)\big)|_{t=1} = \left(\sum_{k=0}^{\infty} \frac{t^k}{k!}\frac{d^k}{ds^k}\omega^{(t)}\big(W(sf)\big)\big|_{s=0}\right)\Bigg|_{t=1} =$$

$$= \sum_{k=0}^{n_0-1} \frac{1}{k!} i^k \omega^{(t)}(\underbrace{f,\ldots,f}_{k \text{ entries}}) \ , \tag{3.23}$$

where in the last step we have used (1.97). We thus conclude from (1.93) that the characteristic function $t \in \mathbb{R} \mapsto \omega\big(W(tf)\big)$ satisfies the hypothesis of Theorem 3.6. Therefore, we have:

$$\omega^{(t)}(\underbrace{f,\ldots,f}_{n \text{ entries}}) = 0 \quad , \qquad \forall\, n \geq 3,\ f \in \mathcal{H}^1 \ . \tag{3.24}$$

We prove the claim by using this identity with

$$f_{\underline{\alpha}} := \sum_{r=1}^{n} e^{i\alpha_r} f_r \ , \tag{3.25}$$

for any

$$\underline{\alpha} = (\alpha_1, \ldots, \alpha_n) \in \mathbb{R}^n \tag{3.26}$$

and arbitrary $f_1, \ldots, f_n \in \mathcal{H}^1$. In particular, we obtain from this:

$$0 = \int_{[0,2\pi]^n} d\alpha_1 \cdots d\alpha_n\, e^{-i(\alpha_1+\cdots+\alpha_n)}\omega^{(t)}(f_{\underline{\alpha}}, \ldots, f_{\underline{\alpha}}) =$$

$$\sum_{r:\{1,\ldots,n\}\to\{1,\ldots,n\}} \omega^{(t)}\left(f_{r(1)}, \ldots, f_{r(n)}\right) \int_{[0,2\pi]^n} d\alpha_1 \cdots d\alpha_n\, e^{-i(\alpha_1+\cdots+\alpha_n)+i(\alpha_{r(1)}+\cdots+\alpha_{r(n)})} \ . \tag{3.27}$$

The value of the integral on the right hand side of this relation is different from zero, if and only if the mapping $r$ is bijective, in which case it equals $(2\pi)^n$. Since

$$\omega^{(t)}(f_{r(1)}, \ldots, f_{r(n)}) = \omega^{(t)}(f_1, \ldots, f_n) \ , \tag{3.28}$$

the claim follows. □

We henceforth restrict our considerations to states $\omega$ with the property that

$$\omega\big(B(f)\big) = 0 \quad , \qquad \forall\ f \in \mathcal{K}\ . \tag{3.29}$$

In order to justify this restriction, we show that to any analytic state $\omega$, obeying certain admissibility conditions, we can pass to an equivalent representation of the many-particle system, such that (3.29) is automatically satisfied.

**Theorem 3.7.** *Let an analytic state $\omega$ and a continuous functional $\varphi : \mathcal{K} \to \mathbb{C}$ with the property*

$$\varphi(\tau\,\cdot\,) = \overline{\varphi(\,\cdot\,)} \tag{3.30}$$

*be given. The unitary implementation $U$ of the Bogoliubov transformation $(\mathbf{1}, \varphi)$ has the property:*

$$\omega\big(UB(f)U^*\big) = \omega\big(B(f)\big) + \varphi(f) \qquad\qquad \forall\ f \in \mathcal{K}\ . \tag{3.31}$$

Note in particular the case:

$$\varphi(f) := -\omega\big(B(f)\big) \quad , \qquad \forall\ f \in \mathcal{K}\ . \tag{3.32}$$

*Proof:* First we point out that $U$ exists by Theorem 2.1, since we have assumed that $\varphi$ is continuous. Next, we prove the lemma for $f \in \mathcal{K}_{\mathbb{R}}$. Recall the definition of the map $\rho : \mathcal{H}^1 \to \mathcal{K}_{\mathbb{R}}$, given in (1.63). It is equivalent to prove

$$\omega\big(U\Phi(g)U^*\big) = \omega\big(\Phi(g)\big) + \varphi\big(\rho(g)\big) \quad , \qquad \forall\ g \in \mathcal{H}^1\ . \tag{3.33}$$

We denote by $\tilde{\omega}$ the state given by

$$\tilde{\omega}(\,\cdot\,) = \omega\big(U(\,\cdot\,)U^*\big)\ . \tag{3.34}$$

It is then easily seen, that

$$\begin{aligned} i\tilde{\omega}\big(\Phi(g)\big) &= \frac{d}{dt}\,\tilde{\omega}\big(W(tg)\big)\big|_{t=0} = \frac{d}{dt}\,e^{i\varphi(\rho(g))t}\cdot\omega\big(W(tg)\big)\big|_{t=0} \\ &= i\varphi\big(\rho(g)\big) + \frac{d}{dt}\omega\big(W(tg)\big)\big|_{t=0} = i\varphi\big(\rho(g)\big) + i\omega\big(\Phi(g)\big)\ . \end{aligned} \tag{3.35}$$

We have used (2.3). This proves (3.33).

Furthermore, for any $f \in \mathcal{K}$, the expectation $\omega\big(B(f)\big)$ may be expressed linearly in terms of expectations of the type $\omega\big(\Phi(g_1)\big)$ and $\omega\big(\Phi(ig_2)\big)$, for some $g_1, g_2 \in \mathcal{H}^1$. This proves the claim. □

### 3.1.2 Generalized Density Matrices

In Appendix A we show how a topology on the Krein space $\mathcal{K}$ may be introduced. The set of everywhere defined operators in $\mathcal{K}$, continuous with respect to this topology, is denoted $\mathcal{B}(\mathcal{K})$. An operator $A$ in $\mathcal{B}(\mathcal{K})$ is called <u>nonnegative in $\mathcal{K}$</u> if

$$[x\,|\,Ax] \geq 0 \quad , \qquad \forall\ x \in \mathcal{K}\ . \tag{3.36}$$

An operator $A \in \mathcal{B}(\mathcal{K})$ is said to be <u>selfadjoint in $\mathcal{K}$</u> if

$$[Ax\,|\,y] = [x\,|\,Ay] \quad , \qquad \forall\ x, y \in \mathcal{K}\ . \tag{3.37}$$

For more details, see Appendix A.

**Definition 3.8.** *A nonnegative operator* $\Gamma$ *in* $\mathcal{B}(\mathcal{K})$ *is called* <u>*generalized density matrix,*</u> *if it obeys*

$$\tau\Gamma\tau = -\mathbf{1} - \Gamma \ . \tag{3.38}$$

*We do not distinguish this operator from the associated quadratic form*

$$\Gamma(f,g) := [f\,|\,\Gamma g] \quad , \qquad \forall\ f,g \in \mathcal{K}\ . \tag{3.39}$$

Similarly to the Hilbert space situation, the non-negativity of a generalized density matrix $\Gamma \in \mathcal{B}(\mathcal{K})$ implies selfadjointness in the Krein space sense by the polarization identity[2]. In this case, relation (3.38) thus translates to the quadratic form $\Gamma(\cdot,\cdot)$, as follows:

$$\Gamma(\tau f, \tau g) = [\tau f\,|\,\Gamma\tau g] = [g\,|\,f] + [\Gamma g\,|\,f] = [g\,|\,f] + \Gamma(g,f) \quad , \qquad \forall\ f,g \in \mathcal{K}\ . \tag{3.41}$$

To any analytic state $\omega$, we associate a generalized density matrix $\Gamma_\omega$ in the following way:

$$\Gamma_\omega(f,g) := \omega\big(B(g)B^*(f)\big) \quad , \qquad \forall\ f,g \in \mathcal{K}\ . \tag{3.42}$$

The definition of the conjugation $\tau$, the properties of $\omega$ as a state and the CCR guarantee that $\Gamma_\omega$ is a generalized density matrix in the sense of the above definition. Furthermore, by restriction to $\mathcal{K}_+$ we recover the usual <u>reduced density matrix</u>[3] $\gamma$:

$$\gamma := P_{\mathcal{K}_+}\Gamma P_{\mathcal{K}_+} \tag{3.44}$$

**Definition 3.9.** *A generalized density matrix* $\Gamma$ *is called an* <u>*admissible generalized density matrix*</u> *if and only if* $\Gamma \in \mathcal{B}(\mathcal{K})$ *and* $\gamma := P_{\mathcal{K}_+}\Gamma P_{\mathcal{K}_+}$ *is trace-class in the Hilbert space* $\mathcal{K}_+$*. In this case* $\mathrm{tr}_{\mathcal{K}_+}(\gamma)$ *is called the* <u>*particle number of*</u> $\Gamma$*. If, additionally,*

$$P_{\mathcal{K}_+}\Gamma P_{\mathcal{K}_-} = P_{\mathcal{K}_-}\Gamma P_{\mathcal{K}_+} = \mathbf{0}\ , \tag{3.45}$$

*then* $\Gamma$ *is said to* <u>*conserve particle number.*</u>

**Definition 3.10.** *An analytic state* $\omega$ *is called an* <u>*admissible state*</u> *if and only if* $\Gamma_\omega$ *is an admissible generalized density matrix and its one-point functional* $f \mapsto \omega\big(a^*(f)\big)$ *is continuous in* $\mathcal{H}^1$*. If, additionally,*

$$\omega\big(a^*(f_1)\cdots a^*(f_n)a(g_1)\cdots a(g_m)\big) = 0\ , \tag{3.46}$$

*for all* $f_1,\cdots,f_n,g_1,\ldots,g_m \in \mathcal{H}^1$ *and* $m \neq n$*, then* $\omega$ *is said to* <u>*conserve particle number.*</u>

We first consider the generalized density matrices conserving the particle number. Note that this condition is equivalent to $\Gamma\mathcal{K}_\pm \subseteq \mathcal{K}_\pm$. By relation (3.38) the generalized density matrix is, in this case, completely determined by $\gamma$.

---

[2]Completely analogous to the Hilbert space situation, we have, for any $A \in \mathcal{B}(\mathcal{K})$ and all $f,g \in \mathcal{K}$,

$$[g\,|\,Af] = \frac{1}{4}\left\{[f+g\,|\,A(f+g)] - [f-g\,|\,A(f-g)] + i\,[f+ig\,|\,A(f+ig)] - i\,[f-ig\,|\,A(f-ig)]\right\}\ . \tag{3.40}$$

[3]Again, we do not distinguish the operator $\gamma$ from the associated quadratic form

$$\gamma(f,g)\ :=\ \langle g\,|\,\gamma f\rangle \qquad \forall\ f,g \in \mathcal{H}^1\ . \tag{3.43}$$

**Proposition 3.11.** *If $\Gamma$ is an admissible generalized density matrix with conserved particle number and $\gamma$ its reduced density matrix, then there exists an admissible, quasi-free state $\omega$, also with conserved particle number, given by*

$$\omega(\,\cdot\,) := \frac{\mathrm{tr}\left(\,\cdot\, Pe^{-\,\mathrm{d}\mathbf{G}(h)}\right)}{\mathrm{tr}\left(Pe^{-\,\mathrm{d}\mathbf{G}(h)}\right)}\ , \tag{3.47}$$

*with*

$$h := P^{\perp}_{\mathrm{kern}\,\gamma}\left(-\ln\frac{\gamma}{1+\gamma}\right)P^{\perp}_{\mathrm{kern}\,\gamma} \qquad \text{and} \qquad P := \mathbf{G}\left(P^{\perp}_{\mathrm{kern}\,h}\right) \tag{3.48}$$

*such that*

$$\Gamma = \Gamma_\omega\ . \tag{3.49}$$

*Proof:* Let a generalized density matrix $\Gamma$ with conserved particle number be given. We first note that the associated reduced density matrix $\gamma$ possesses a complete orthonormal set $\{f_j\}_{j\in J}$ of eigenvectors, since it is a trace-class operator in the Hilbert space $\mathcal{K}_+$. To each such $f_j$ corresponds an eigenvalue of $\gamma$ denoted by $\gamma_j$. For the purpose of this proof, we introduce

$$J' \ :=\ \big\{\, j\in J \mid \gamma_j > 0\,\big\}\ . \tag{3.50}$$

According to the definition of $P$ and (1.15) we have

$$P\big(\mathcal{S}_+ f_{j_1}\otimes\cdots\otimes f_{j_N}\big) := \begin{cases} \mathcal{S}_+ f_{j_1}\otimes\cdots\otimes f_{j_N} & \text{if } j_1,\ldots,j_N\in J' \\ 0 & \text{else}\end{cases}\ . \tag{3.51}$$

We now demonstrate that (3.47) defines an appropriate quasi-free state.

First, we must show that $\omega$ is well-defined, by proving that $Pe^{-\,\mathrm{d}\mathbf{G}(h)}$ is trace-class. Before doing so, let us quote a special case of statement (3.157):

$$\mathrm{tr}\left(Pe^{-\sum_{j\in J'}\lambda_j a^*(f_j)a(f_j)}\right) = \prod_{j\in J'}\frac{1}{1-e^{-\lambda_j}}\ , \quad \text{provided} \qquad \sum_{j\in J'}\frac{e^{-\lambda_j}}{1-e^{-\lambda_j}} < \infty\ . \tag{3.52}$$

The assumption of finiteness imposed on the family $\{\lambda_j\}_{j\in J}$ in (3.52) guarantees the existence and finiteness of the infinite product (for a review on the theory of convergence of infinite products, see e. g. [33]). On setting $\lambda_j = -\ln\frac{\gamma_j}{1+\gamma_j}$, according to (3.47), for all $j\in J'$, the well-definedness of $\omega$ follows. This is because the condition of finiteness in relation (3.52) is equivalent to the trace-class condition on $\gamma$. It remains to prove that the state we have thus constructed has $\Gamma$ as its generalized density matrix. To this end we note that the state $\omega$ is analytic, due to Theorem 3.22. We have due to (3.52)

$$\begin{aligned}\omega\big(a^*(f_j)a(f_k)\big) &= -\delta_{j,k}\frac{\partial}{\partial\lambda_j}\ln\mathrm{tr}\left(Pe^{-\sum_{j\in J'}\lambda_j a^*(f_j)a(f_j)}\right)\\ &= -\delta_{j,k}\frac{e^{-\lambda_j}}{1-e^{-\lambda_j}} = \delta_{j,k}\gamma_j\ ,\end{aligned} \tag{3.53}$$

for all $j,k\in J'$, and hence, we have $\gamma(f,g) = \omega\big(a^*(g)a(f)\big)$, for all $f,g\in\mathcal{K}_+$. From Lemma D.1 and Theorem 3.22 we deduce that the constructed state $\omega$ is quasi-free, by noting that the hierarchy $\omega^{(t)}$ has vanishing $n$-point functions, whenever $n\geq 3$. $\square$

We generalize Proposition 3.11 to all admissible generalized density matrices on the basis of the following diagonalization lemma, which we prove in Appendix A, and Lemma 3.13 saying that the Bogoliubov transformation diagonalizing $\Gamma$ is unitarily implementable.

**Lemma 3.12.** *To any admissible generalized density matrix $\Gamma$, there exists a self-dual fundamental decomposition (see Definition A.2) $\mathcal{K} = \tilde{\mathcal{K}}_+ {}^{[+]} \tilde{\mathcal{K}}_-$ such that*

$$\Gamma\tilde{\mathcal{K}}_+ \subseteq \tilde{\mathcal{K}}_+ \ . \tag{3.54}$$

*Proof:* See Lemma A.9. □

Assume the hypothesis of the above lemma is satisfied. As we have demonstrated in Subsection 1.1.3, we may then find a homogeneous Bogoliubov transformation $w$, such that $w\!\restriction_{\mathcal{K}_\pm}$ maps the Hilbert spaces $\mathcal{K}_\pm$ unitarily onto the Hilbert spaces $\tilde{\mathcal{K}}_\pm$. (The fact that $\tilde{\mathcal{K}}_\pm$ are also Hilbert spaces with respect to the scalar products $\pm[\cdot\,|\,\cdot]\restriction_{\tilde{\mathcal{K}}_\pm}$ is shown in Theorem A.4.) Its properties are the subject matter of the following lemma.

**Lemma 3.13.** *If $\Gamma$ is an admissible generalized density matrix and $w$ is an homogeneous Bogoliubov transformation mapping the invariant subspaces $\tilde{\mathcal{K}}_\pm$ of $\Gamma$ onto the subspaces $\mathcal{K}_\pm$, then the following defines an admissible generalized density matrix $\tilde{\Gamma}$:*

$$\tilde{\Gamma} := w\Gamma w^{[*]} \ . \tag{3.55}$$

*Moreover, the transformation $w$ has a unitary implementation in $\mathcal{F}_+$.*

$w^{[*]}$ denotes the adjoint of $w$ with respect to the inner product $[\cdot\,|\,\cdot]$ in $\mathcal{K}$, see Section A.2.

*Proof:* Evidently, $\tilde{\Gamma}$ is a generalized density matrix. In order to prove its admissibility we note: With respect to the fundamental decomposition $\mathcal{K} = \mathcal{K}_+ {}^{[+]} \mathcal{K}_-$, we may write $\Gamma$ and $\tilde{\Gamma}$ as $2\times 2$ block matrices in the following way

$$\Gamma = \begin{pmatrix} \gamma & \alpha \\ -\bar{\alpha} & -\mathbf{1}-\bar{\gamma} \end{pmatrix} , \qquad \tilde{\Gamma} = w\Gamma w^{[*]} =: \begin{pmatrix} \tilde{\gamma} & \mathbf{0} \\ \mathbf{0} & -\mathbf{1}-\bar{\tilde{\gamma}} \end{pmatrix} , \tag{3.56}$$

for some operators $\tilde{\gamma}$, $\gamma$ and $\alpha$ in $\mathcal{H}^1$. By the properties of $\Gamma$ we have that $\gamma \geq 0$ is trace-class and that $\alpha^T = \alpha$. Similarly we have $\tilde{\gamma} \geq 0$, since $w$ is unitary in $\mathcal{K}$, see (A.22). Since the trace[4] is cyclic and by relation (2.2), we have

$$\mathrm{tr}\left(\tilde{\Gamma}(\mathbf{1}+\tilde{\Gamma})\right) = \mathrm{tr}\left(\Gamma(\mathbf{1}+\Gamma)\right) \ . \tag{3.57}$$

Reexpressing[5] this equation in terms of $\alpha$, $\gamma$ and $\tilde{\gamma}$, we obtain

$$\mathrm{tr}(\tilde{\gamma}^2) + \mathrm{tr}(\tilde{\gamma}) + \mathrm{tr}(\alpha\alpha^*) = \mathrm{tr}(\gamma^2) + \mathrm{tr}(\gamma) < \infty \ , \tag{3.58}$$

[4]We can introduce on $\mathcal{K}$ the scalar product given by

$$\langle f\,|\,g\rangle_{\mathcal{K}} := \langle f^+\,|\,g^+\rangle + \langle f^-\,|\,g^-\rangle \quad , \qquad \forall\ f,g\in\mathcal{K}\ .$$

The above trace is defined with respect to the Hilbert space $(\mathcal{K}, \langle\cdot\,|\,\cdot\rangle_{\mathcal{K}})$.

[5]Note that $\mathcal{K} = \mathcal{K}_+ \oplus \mathcal{K}_-$ is also orthogonal with respect to $\langle\cdot\,|\,\cdot\rangle_{\mathcal{K}}$. (See Footnote 4).

implying the trace-class property of $\tilde{\gamma}$ and hence the admissibility of $\tilde{\Gamma}$. Moreover, it follows that $\alpha$ is Hilbert-Schmidt[6]. We now prove that $w$ possesses a unitary implementation: On writing the Bogoliubov transformation $w$, like we have done with the generalized density matrices in (3.56), as a block matrix, it has the form (2.6), for some operators $X$ and $Y$ in $\mathcal{B}(\mathcal{H}^1)$. (The boundedness follows from the fact, that any unitary transformation in a Krein space is bounded, see Theorem A.4.) Therefore, we have, by (3.56),

$$\tilde{\gamma} = X\gamma X^* - Y\bar{\alpha}X^* - X\alpha Y^* + Y(\mathbf{1}+\bar{\gamma})Y^* \tag{3.59}$$

and hence

$$\begin{aligned}\infty > \operatorname{tr}(\tilde{\gamma}) &= \operatorname{tr}(X^*X\gamma) - \operatorname{tr}(Y\bar{\alpha}X^*) - \operatorname{tr}(X\alpha Y^*) + \operatorname{tr}(YY^*) + \operatorname{tr}(Y^*Y\bar{\gamma}) \\ &\geq \operatorname{tr}\big((X^*X - Y^T\bar{Y})\gamma\big) - \operatorname{tr}(Y\bar{\alpha}X^*) - \operatorname{tr}(X\alpha Y^*) + \operatorname{tr}(YY^*) \\ &= \operatorname{tr}(\gamma) - \operatorname{tr}(Y\bar{\alpha}X^*) - \operatorname{tr}(X\alpha Y^*) + \operatorname{tr}(YY^*)\ .\end{aligned} \tag{3.60}$$

In the last step we use relations (2.7). Applying the Cauchy-Schwarz inequality, we estimate

$$\big|\operatorname{tr}(Y^T\bar{\alpha}X)\big|, \big|\operatorname{tr}(Y\bar{\alpha}X^*)\big| \leq \sqrt{\operatorname{tr}(XX^*\alpha\alpha^*)\operatorname{tr}(\bar{Y}Y^T)}\ , \tag{3.61}$$

where we additionally use $\bar{\alpha} = \alpha^*$, to obtain

$$\begin{aligned}\infty &> \operatorname{tr}(\gamma) - 2\sqrt{\operatorname{tr}(XX^*\alpha\alpha^*)\operatorname{tr}(\bar{Y}Y^T)} + \operatorname{tr}(YY^*) \\ &= \operatorname{tr}(\gamma) + \Big(\sqrt{\operatorname{tr}(Y^*Y)} - \sqrt{\operatorname{tr}(XX^*\alpha\alpha^*)}\Big)^2 - \operatorname{tr}(XX^*\alpha\alpha^*)\ .\end{aligned} \tag{3.62}$$

Since $\gamma$ is, as we have pointed out, a trace-class operator and furthermore $\alpha$ is Hilbert-Schmidt, it follows that $\operatorname{tr}(YY^*) = \operatorname{tr}(\bar{Y}Y^T) < \infty$. By Theorem 2.1, this proves that $w$ possesses a unitary implementation. $\square$

Proposition 3.11 together with Lemmas 3.12 and 3.13 proves:

**Proposition 3.14.** *If $\Gamma$ is an admissible generalized density matrix, then there is an admissible quasi-free state $\omega$ conserving the number of particles such that*

$$\Gamma_\omega = \Gamma\ . \tag{3.63}$$

We now proceed to prove the 1:1-correspondence between admissible quasi-free states, with one-point functions possibly not vanishing, and generalized density matrices. This correspondence is given by assigning to any admissible state $\omega$ a so-called admissible pair $(\Gamma, v)$ consisting of a generalized density matrix and a functional $v : \mathcal{K} \to \mathbb{C}$. The functional $v$ is supposed to carry the information on the one-point function of the state.

By Theorem 3.7, any admissible state $\omega$ may be transformed by the inhomogeneous Bogoliubov transformation $\big(\mathbf{1}_\mathcal{K}, -\omega(B(\cdot))\big)$, possessing a unitary implementation $U$, into a state $\tilde{\omega}(\cdot) := \omega(U^* \cdot U)$ with vanishing one-point function. The two-point function of this state has the property

$$\tilde{\omega}\big(B(f)B^*(f)\big) = \omega\big(B(f)B^*(f)\big) - \big|\,\omega\big(B(f)\big)\,\big|^2\ , \tag{3.64}$$

for all $f \in \mathcal{K}$. This motivates the following definition.

[6]It may come as a little surprise that the Hilbert-Schmidt property of $\alpha$ follows at this stage of the argument. In Remark 3.17 at the end of this subsection we show, however, how this can be seen *a priori*, for all admissible generalized density matrices.

**Definition 3.15.** *A pair* $(\Gamma, v)$ *consisting of an admissible generalized density matrix* $\Gamma$ *and a continuous functional* $v : \mathcal{K} \to \mathbb{C}$*, called* <u>*one-point functional*</u>*, with the additional property* $v(\tau\,\cdot\,) = \overline{v(\,\cdot\,)}$*, is called an* <u>*admissible pair*</u>*, if*

$$\tilde{\Gamma}(f, g) := \Gamma(f, g) - \overline{v(f)}v(g) \qquad \forall\ f, g \in \mathcal{K} \tag{3.65}$$

*is a nonnegative quadratic form, i. e., if*

$$\tilde{\Gamma}(f, f) \geq 0 \quad , \qquad \forall\ f \in \mathcal{K}\ . \tag{3.66}$$

It is easy to see, that the quadratic form $\tilde{\Gamma}(f, g)$ defined in (3.65) is again a generalized density matrix by verifying (3.41). Furthermore, defining a linear structure on the set of admissible pairs, by setting

$$z_1(\Gamma_1, v_1) + z_2(\Gamma_2, v_2) := (z_1\Gamma_1 + z_2\Gamma_2,\ z_1v_1 + z_2v_2) \quad , \qquad \forall\ z_1, z_2 \in \mathbb{R}_0^+\ , \tag{3.67}$$

we see that the set of admissible pairs is a convex set, because

$$\begin{aligned} &\lambda\Gamma_1(f, f) + (1-\lambda)\Gamma_2(f, f) - |\,\lambda v_1(f) - (1-\lambda)v_2(f)\,|^2 \\ &\qquad \geq \lambda\Gamma_1(f, f) - \lambda\,|\,v_1(f)\,|^2 + (1-\lambda)\Gamma_2(f, f) - (1-\lambda)\,|\,v_2(f)\,|^2 \geq 0\ , \end{aligned} \tag{3.68}$$

for any two admissible pairs $(\Gamma_1, v_1)$ and $(\Gamma_2, v_2)$ and any $\lambda \in (0, 1)$, by the simple fact that $z \mapsto |\,z\,|^2$ is convex. We shall now show that the admissible pairs are in 1:1-correspondence to the admissible quasi-free states.

**Theorem 3.16.** *The mapping*

$$\omega \mapsto (\Gamma_\omega, v_\omega)\ , \quad \textit{with} \qquad v_\omega(\cdot) := \omega\big(B(\cdot)\big) \qquad \textit{and} \qquad (3.42) \tag{3.69}$$

*bijectively assigns to each admissible quasi-free state an admissible pair.*

*Proof:* It is clear that the mapping (3.69) is injective, since $\omega$ is completely determined by its one-point and two-point functions.

To prove surjectivity, we construct the right inverse of the mapping $\omega \mapsto (\Gamma_\omega, v_\omega)$. To this end, let an admissible pair $(\Gamma, v)$ be given. The quadratic form $\tilde{\Gamma}$ given by

$$\tilde{\Gamma}(f, g) := \Gamma(f, g) - \overline{v(f)}v(g) \quad , \qquad \forall\ f, g \in \mathcal{K}\ , \tag{3.70}$$

is then an admissible generalized density matrix. To see this, use relation (3.41). As we have seen in Proposition 3.14, we are able to construct a quasi-free state $\tilde{\omega}$ with the properties

$$\tilde{\omega}\big(B(g)B^*(f)\big) = \tilde{\Gamma}(f, g) \tag{3.71}$$

and

$$\tilde{\omega}\big(B(f)\big) = 0\ , \tag{3.72}$$

for all $f, g \in \mathcal{K}$. Let us now set $\omega := \tilde{\omega}(U(\,\cdot\,)U^*)$, where $U$ denotes the unitary implementation of the Bogoliubov transformation $(\mathbf{1}, v)$. By Theorem 3.7 we thus have

$$\omega\big(B(f)\big) = v(f) \quad , \qquad \forall\ f \in \mathcal{K}\ . \tag{3.73}$$

Furthermore, we remark that, for all $f, g \in \mathcal{H}^1$, we have:

$$\begin{aligned}\omega\big(\Phi(g)\Phi(f))\big) &= -\frac{\partial}{\partial t_1}\frac{\partial}{\partial t_2}\tilde{\omega}\big(UW(t_1 g)W(t_2 f)U^*\big)|_{t_1=t_2=1} \\ &= -\frac{\partial}{\partial t_1}\frac{\partial}{\partial t_2}e^{i(t_1\cdot v(\rho(f))+t_2\cdot v(\rho(g)))}\tilde{\omega}\big(W(t_1 g)W(t_2 f)\big)|_{t_1=t_2=0} \\ &= v(f)v(g) + \tilde{\omega}\big(\Phi(g)\Phi(f)\big) \ ,\end{aligned}$$

using (2.3) and (1.63). (Note that in the last step we have used (3.72).) This implies $\omega\big(B(g)B^*(f)\big) = \Gamma(f,g)$ by (3.70) and thus completes the proof. □

**Remark 3.17:** As in (3.56), let $\Gamma$ be a generalized density matrix in $\mathcal{B}(\mathcal{K})$ and suppose $\Gamma$ has the form

$$\Gamma = \begin{pmatrix} \gamma & \alpha \\ -\bar{\alpha} & -\mathbf{1}-\bar{\gamma} \end{pmatrix} \ , \tag{3.74}$$

for some $\alpha$ and some $\gamma$ with respect to the fundamental decomposition (1.53). It is easy to see that, if $\Gamma$ is the generalized density matrix of some analytic state $\omega$, then $\gamma$ and $\alpha$ are determined by

$$\langle f \,|\, \gamma g\rangle = \omega\big(a^*(g)a(f)\big) \qquad \text{and} \qquad \langle f \,|\, \alpha g\rangle = \omega\big(a(\bar{g})a(f)\big) \quad , \qquad \forall\ f, g \in \mathcal{H}^1. \tag{3.75}$$

Define $\Gamma'$ to be the operator in $\mathcal{K}$ given by

$$\Gamma' = \begin{pmatrix} \gamma & \alpha \\ \bar{\alpha} & \mathbf{1}+\bar{\gamma} \end{pmatrix} \ . \tag{3.76}$$

Note that $\Gamma'$ is a nonnegative operator in the Hilbert (!) space $(\mathcal{K}, \langle\cdot\,|\,\cdot\rangle_{\mathcal{K}})$, where

$$\langle f \,|\, g\rangle_{\mathcal{K}} \ := \ \langle f^+ \,|\, g^+\rangle_{\mathcal{H}^1} + \langle f^- \,|\, g^-\rangle_{\mathcal{H}^1} \quad , \qquad \forall\ f, g \in \mathcal{K} \ .$$

If $\Gamma$ is admissible, then $\gamma$ is bounded, and by nonnegativity $\Gamma'$ is also bounded as an operator in $(\mathcal{K}, \langle\cdot\,|\,\cdot\rangle_{\mathcal{K}})$. Hence we have $(\Gamma')^2 \leq \|\,\Gamma'\,\|\,\Gamma'$ with respect to $\langle\cdot\,|\,\cdot\rangle_{\mathcal{K}}$. From the left upper block of this inequality, we obtain, for all admissible generalized density matrices of the form (3.74), that $\alpha$ is Hilbert-Schmidt.

### 3.1.3 Quadratic Operators

In this subsection, we discuss selfadjoint operators in $\mathcal{F}_+$, which can be expressed quadratically in terms of the boson particle creation and annihilation operators $a^*(\cdot)$ and $a(\cdot)$. Let $\{f_k\}_{k\in\mathbb{N}}$ be an orthonormal basis in $\mathcal{H}^1$. Namely, we consider operators $H$ of the form

$$H := \mathrm{d}\mathbf{G}(c) + \sum_{k,k'\in I}\big(b_{k,k'}a^*(f_k)a^*(\bar{f}_{k'}) + \bar{b}_{k,k'}a(\bar{f}_k)a(f_{k'})\big) + \Phi(g) \ , \tag{3.77}$$

for some selfadjoint operator $c$ in $\mathcal{H}^1$, some *finite* index set $I$, arbitrary numbers $\{b_{k,k'}\}_{k,k'\in I}$ with $b_{k,k'} = b_{k',k}$, and some $g \in \mathcal{H}^1$. We define $H$ on the domain

$$D := F_+ \ \cap \ \mathcal{D}\big(\mathrm{d}\mathbf{G}(c)\big) \ . \tag{3.78}$$

By Theorem 1.2, it is clear that $D$ is dense in $\mathcal{F}_+$. Note that

$$A_n^+ : \mathcal{H}_+^n \to \mathcal{F}_+ \ , \quad \text{with} \qquad A_n^+\psi := \sum_{k,k' \in I} b_{k,k'} a^*(f_k) a^*(\bar{f}_{k'})\psi \ , \tag{3.79a}$$

is, for any $n \in \mathbb{N}$, a bounded operator. Completely analogous,

$$A_n^- : \mathcal{H}_+^n \to \mathcal{F}_+ \ , \quad \text{with} \qquad A_n^-\psi := \sum_{k,k' \in I} b_{k,k'} a(\bar{f}_k) a(f_{k'})\psi \tag{3.79b}$$

is, for all $n \in \mathbb{N}_0$, also a bounded operator. We prove a simplified version of Theorem 6.1 in [10].

**Theorem 3.18.** *The operator $H$ in $\mathcal{F}_+$ defined in* (3.77) *is essentially selfadjoint on the domain $D$ given in* (3.78).

*Proof:* We denote by $D^*$ the domain of $H^*$. The first step we take, is to show that

$$D^* \cap \mathcal{H}_+^n \ \subseteq \ \mathcal{D}\big(\,\mathrm{d}\mathbf{G}(c)\big) \cap \mathcal{H}_+^n \quad , \qquad \forall\, n \in \mathbb{N}_0 \ . \tag{3.80}$$

Assume that $\phi^{(n)} \in D^* \cap \mathcal{H}_+^n$, for arbitrary $n \in \mathbb{N}_0$. It then follows that

$$\infty > \sup_{\psi \in D \setminus \{0\}} \frac{\big|\,\big\langle \phi^{(n)} \,\big|\, H\psi \big\rangle\,\big|}{\|\,\psi\,\|} \ . \tag{3.81}$$

Taking the supremum over the smaller set $D_n := D \cap \mathcal{H}_+^n$, estimates the right hand side of this relation from below. Thus we obtain:

$$\begin{aligned} \infty > \sup_{\psi^{(n)} \in D_n \setminus \{0\}} \frac{\big|\,\big\langle \phi^{(n)} \,\big|\, H\psi^{(n)} \big\rangle\,\big|}{\|\,\psi^{(n)}\,\|} &= \sup_{\psi^{(n)} \in D_n \setminus \{0\}} \frac{\big|\,\big\langle \phi^{(n)} \,\big|\, \mathrm{d}\mathbf{G}(c)\psi^{(n)} \big\rangle\,\big|}{\|\,\psi^{(n)}\,\|} \\ \geq \sup_{\psi \in \mathcal{D}(\mathrm{d}\mathbf{G}(c)) \setminus \{0\}} \frac{\big|\,\big\langle \phi^{(n)} \,\big|\, \mathrm{d}\mathbf{G}(c)\psi \big\rangle\,\big|}{\|\,\psi\,\|} \ . \end{aligned} \tag{3.82}$$

In the second last step we have exploited the fact that $\big\langle \phi^{(n)} \,\big|\, H\psi^{(n)} \big\rangle = \big\langle \phi^{(n)} \,\big|\, \mathrm{d}\mathbf{G}(c)\psi^{(n)} \big\rangle$, for all $\psi \in \mathcal{D}\big(\,\mathrm{d}\mathbf{G}(c)\big)$ and all $n \in \mathbb{N}_0$. Thus it follows that

$$\phi^{(n)} \in \mathcal{D}\big(\,\mathrm{d}\mathbf{G}(c)\big) \ , \tag{3.83}$$

proving (3.80). Let us now recall definitions (3.79). Furthermore, we set for all $n \in \mathbb{N}_0$:

$$F_n^+ : \mathcal{H}_+^n \to \mathcal{F}_+ \ , \qquad \text{with} \qquad F_n^+\psi := \frac{1}{\sqrt{2}} a^*(g_1)\psi \ , \tag{3.84}$$

$$F_n^- : \mathcal{H}_+^n \to \mathcal{F}_+ \ , \qquad \text{with} \qquad F_n^-\psi := \frac{1}{\sqrt{2}} a(\bar{g}_1)\psi \ . \tag{3.85}$$

For any $n \in \mathbb{N}_0$, $F_n^\pm$ are defined on $\mathcal{H}_+^n$ and these operators are bounded. It is now easily seen by (3.80) that

$$\Big\langle \phi^{(n)} \,\big|\, H\psi \Big\rangle = \Big\langle \mathrm{d}\mathbf{G}(c)\phi^{(n)} + A_n^+\phi^{(n)} + A_n^-\phi^{(n)} + F_n^+\phi^{(n)} + F_n^-\phi^{(n)} \,\big|\, \psi \Big\rangle \ , \tag{3.86}$$

for any $\phi \in D^*$, any $\psi \in D$ and all $n \in \mathbb{N}_0$. Hence we have:

$$H^* \phi^{(n)} = \mathrm{d}\mathbf{G}(c)\phi^{(n)} + A_n^+ \phi^{(n)} + A_n^- \phi^{(n)} + F_n^+ \phi^{(n)} + F_n^- \phi^{(n)} \ , \tag{3.87}$$

for all $n \in \mathbb{N}_0$ and all $\phi \in D^*$.

Following Carleman [14] we now show that, for $H$ to have both deficiency indices equal to zero, it is sufficient that

$$\sum_{n=1}^{\infty} \frac{1}{\max\{\| A_{n-1}^+ \| , \| A_n^+ \| , \| F_n^+ \|\}} = \infty \ . \tag{3.88}$$

Suppose that, for some $z \in \mathbb{C}$ and some $\phi \in D^* \setminus \{0\}$, we had

$$H^* \phi = z \cdot \phi \ . \tag{3.89}$$

It then follows from (3.87), for all $k \in \mathbb{N}_0$:

$$z \cdot \phi^{(k)} = \mathrm{d}\mathbf{G}(c)\phi^{(k)} + A_{k-2}^+ \phi^{(k-2)} + A_{k+2}^- \phi^{(k+2)} + F_{k-1}^+ \phi^{(k-1)} + F_{k+1}^- \phi^{(k+1)} \ , \tag{3.90}$$

where we have additionally set

$$A_{-k}^{\pm} \phi^{(-k)} := 0 \qquad \text{and} \qquad F_{-k}^{\pm} \phi^{(-k)} := 0 \quad , \qquad \forall\, k \in \mathbb{N} \ . \tag{3.91}$$

From (3.90) we may conclude:

$$\begin{aligned} 2\,\mathrm{Im}(z) \left\| \phi^{(k)} \right\|^2 = & \left\langle \phi^{(k)} \,\middle|\, A_{k-2}^+ \phi^{(k-2)} \right\rangle + \left\langle \phi^{(k)} \,\middle|\, A_{k+2}^- \phi^{(k+2)} \right\rangle \\ & + \left\langle \phi^{(k)} \,\middle|\, F_{k-1}^+ \phi^{(k-1)} \right\rangle + \left\langle \phi^{(k)} \,\middle|\, F_{n+1}^- \phi^{(k+1)} \right\rangle \\ & - \left\langle \phi^{(k-2)} \,\middle|\, A_k^- \phi^{(k)} \right\rangle - \left\langle \phi^{(k+2)} \,\middle|\, A_k^+ \phi^{(k)} \right\rangle \\ & - \left\langle \phi^{(k-1)} \,\middle|\, F_k^- \phi^{(k)} \right\rangle - \left\langle \phi^{(k+1)} \,\middle|\, F_k^+ \phi^{(k)} \right\rangle \ , \end{aligned} \tag{3.92}$$

where we have used

$$\left\langle \phi^{(k\pm2)} \,\middle|\, A_k^{\pm} \phi^{(k)} \right\rangle = \left\langle A_{k\pm2}^{\mp} \phi^{(k\pm2)} \,\middle|\, \phi^{(k)} \right\rangle \ , \tag{3.93a}$$

$$\left\langle \phi^{(k\pm1)} \,\middle|\, F_k^{\pm} \phi^{(k)} \right\rangle = \left\langle F_{k\pm1}^{\mp} \phi^{(k\pm1)} \,\middle|\, \phi^{(k)} \right\rangle \ , \tag{3.93b}$$

for all $\phi \in \mathcal{F}_+$ and all $k \in \mathbb{N}_0$. Summing up (3.92) for all $k \in \{0, \ldots, n\}$, yields the following identity:

$$\begin{aligned} 2\,\mathrm{Im}(z) \sum_{k=0}^{n} \left\| \phi^{(k)} \right\|^2 = & \left\langle \phi^{(n-1)} \,\middle|\, A_{n+1}^- \phi^{(n+1)} \right\rangle + \left\langle \phi^{(n)} \,\middle|\, A_{n+2}^- \phi^{(n+2)} \right\rangle \\ & - \left\langle \phi^{(n+1)} \,\middle|\, A_{n-1}^+ \phi^{(n-1)} \right\rangle - \left\langle \phi^{(n+2)} \,\middle|\, A_n^+ \phi^{(n)} \right\rangle \\ & + \left\langle \phi^{(n)} \,\middle|\, F_{n+1}^- \phi^{(n+1)} \right\rangle - \left\langle \phi^{(n+1)} \,\middle|\, F_n^+ \phi^{(n)} \right\rangle \ . \end{aligned} \tag{3.94}$$

Using the Cauchy-Schwarz estimate and the elementary estimate

$$2ab \leq a^2 + b^2 \quad , \qquad \forall\, a, b \in \mathbb{R} \ , \tag{3.95}$$

we obtain

$$2\,|\,\mathrm{Im}(z)\,|\sum_{k=0}^{n}\left\|\,\phi^{(k)}\,\right\|^{2}\leq\max\{\|\,A_{n-1}^{+}\,\|\,,\|\,A_{n}^{+}\,\|\,,\|\,F_{n}^{+}\,\|\}$$
$$\cdot\left(\left\|\,\phi^{(n-1)}\,\right\|^{2}+\left\|\,\phi^{(n+2)}\,\right\|^{2}+2\left\|\,\phi^{(n)}\,\right\|^{2}+2\left\|\,\phi^{(n+1)}\,\right\|^{2}\right)\ . \tag{3.96}$$

Since $\phi$ is assumed to be nontrivial, we have

$$\left\|\,\phi^{(n-1)}\,\right\|^{2}+\left\|\,\phi^{(n+2)}\,\right\|^{2}+2\left\|\,\phi^{(n)}\,\right\|^{2}+2\left\|\,\phi^{(n+1)}\,\right\|^{2}$$
$$\geq\frac{2\,|\,\mathrm{Im}(z)\,|\,\mu}{\max\{\|\,A_{n-1}^{+}\,\|\,,\|\,A_{n}^{+}\,\|\,,\|\,F_{n}^{+}\,\|\}}\quad,\qquad\forall\ n\geq n_0\ , \tag{3.97}$$

for $\mu>0$ and $n_0\geq 1$ chosen such that

$$\mu=\sum_{k=0}^{n_0}\left\|\,\phi^{(k)}\,\right\|^{2}>0\ . \tag{3.98}$$

Summing up over all $n\in\mathbb{N}$ with $n\geq n_0$ and supplementing the missing terms on the left hand side, we obtain

$$3\,\|\,\phi\,\|^{2}\geq|\,\mathrm{Im}(z)\,|\,\mu\sum_{n=n_0}^{\infty}\frac{1}{\max\{\|\,A_{n-1}^{+}\,\|\,,\|\,A_{n}^{+}\,\|\,,\|\,F_{n}^{+}\,\|\}}\ . \tag{3.99}$$

Thus (3.88) suffices to show that (3.89) possesses no nontrivial solutions for $z\in\mathbb{C}\setminus\mathbb{R}$, implying that both deficiency indices of $H$ are then equal to zero.

In order to complete the proof of the theorem, it just remains to show that (3.88) holds. As we have already remarked, the operators $A_n^+$ and $F_n^+$ are bounded, for all $n\in\mathbb{N}$. More precisely, we have for any $n\in\mathbb{N}$

$$\|\,A_n^{+}\,\|\leq a\sqrt{(n+1)(n+2)}\qquad\text{and}\qquad\|\,F_n^{+}\,\|\leq a\sqrt{n+1}\ , \tag{3.100}$$

for some finite constant $a$ independent of $n$, by Theorem 1.3. Thus, for sufficiently large $n$, we have

$$\frac{1}{\max\{\|\,A_{n-1}^{+}\,\|\,,\|\,A_{n}^{+}\,\|\,,\|\,F_{n}^{+}\,\|\}}\geq\frac{1}{a\sqrt{(n+1)(n+2)}}\ . \tag{3.101}$$

Since the right hand side of this estimate is not summable, (3.88) holds, proving the claim. □

**Remark 3.19:** It would be desirable to allow in (3.77) for a countably infinite index set $I$, demanding instead

$$\sum_{k,k'\in I}\left|\,b_{k,k'}\,\right|^{2}<\infty\ . \tag{3.102}$$

In this case, however, it is not clear if the operators

$$\sum_{k,k'\in I}b_{k,k'}a^{*}(f_k)a^{*}(\bar{f}_{k'})\qquad\text{and}\qquad\sum_{k,k'\in I}\bar{b}_{k,k'}a(\bar{f}_k)a(f_{k'}) \tag{3.103}$$

are both defined on $\mathcal{H}_+^n$, for all $n \in \mathbb{N}$. Furthermore, it is not obvious that (3.93) hold. Unless these questions can be clarified, the above argument is, in the case of an infinite $I$, just formal.

Henceforth, we view all quadratic expressions of the form (3.77), as selfadjoint operators in $\mathcal{F}_+$ invoking Theorem 3.18.

Consider the same orthonormal set $\{f_k\}_{k\in\mathbb{N}}$ introduced at the beginning of this subsection as a set of vectors in $\mathcal{K}_+ \subseteq \mathcal{K}$ and define

$$f_{-k} := \tau f_k \quad , \qquad \forall\, k \in \mathbb{N}\ . \tag{3.104}$$

Then the set $\{f_k\}_{k\in K}$, with $K := \mathbb{N} \cup (-\mathbb{N})$, has the following orthogonality property

$$[f_k \,|\, f_{k'}] = \mathrm{sign}(k) \cdot \delta_{k,k'} \quad , \qquad \forall\, k, k' \in K\ . \tag{3.105}$$

Such a total set of vectors is called a <u>self-dual basis in $\mathcal{K}$</u>. In terms of this self-dual basis, we can reexpress $H$ in the following form

$$H = \sum_{k,k'\in K} [f_k \,|\, M f_{k'}]\, B(f_k) B^*(f_{k'}) + \Phi(g)\ , \tag{3.106}$$

where $M$ is the $2 \times 2$-block-matrix given by

$$M = \begin{pmatrix} c & -b \\ b^* & \mathbf{0} \end{pmatrix} \tag{3.107}$$

and $b$ is the finite rank operator in $\mathcal{H}^1$ given by

$$\langle f_k \,|\, b f_{k'} \rangle := b_{k,k'} \quad , \qquad \forall\, k, k' \in \mathbb{N}\ . \tag{3.108}$$

(The numbers $b_{k,k'}$ are assumed to be zero for $k \notin I$ or $k' \notin I$.)

It is now easy to express the action of a homogeneous Bogoliubov transformation $w$, possessing a unitary implementation $U_w$ in $\mathcal{F}_+$, as a transformation of the matrix $M$. Namely, if $w$ is a homogeneous Bogoliubov transformation and $U_w H U_w^*$ is the corresponding transform of the quadratic operator $H$, we have:

$$U_w H U_w^* = \sum_{k,k'\in K} \left[ \tilde{f}_k \,\middle|\, w M w^{[*]} \tilde{f}_{k'} \right] B(\tilde{f}_k) B^*(\tilde{f}_{k'}) + \Phi\big(\rho^{-1}(w\rho(g))\big) \tag{3.109}$$

with $\tilde{f}_k := w f_k$, for all $k \in K$. Recall (1.63). Note that $\{\tilde{f}_k\}_{k\in K}$ is a self-dual basis of $\mathcal{K}$ with respect to the fundamental decomposition

$$\mathcal{K} = \tilde{\mathcal{K}}_+ {}^{[+]}\, \tilde{\mathcal{K}}_-\ , \qquad \text{with} \qquad \tilde{\mathcal{K}}_\pm := w\mathcal{K}_\pm\ . \tag{3.110}$$

We now show, how the generators $B(\cdot)$ of the self-dual CCR Algebra transform under the action of the strongly continuous groups generated by quadratic operators $H = H^*$.

**Theorem 3.20.** *Let $H$ be a selfadjoint operator in $\mathcal{F}_+$ of the form (3.106) and assume that there exists a homogeneous Bogoliubov transformation $w$, possessing a unitary implementation $U_w$, such that*

$$\tilde{H} := U_w H U_w^* = \mathrm{d}\mathbf{G}(c) \ , \tag{3.111}$$

*for some one-particle operator $c = c^*$ in $\mathcal{B}(\mathcal{H}^1)$. Then the operators*

$$C := \begin{pmatrix} c & \mathbf{0} \\ \mathbf{0} & -\bar{c} \end{pmatrix} \qquad \text{and} \qquad M - \tau M \tau = w^{[*]} C w \tag{3.112}$$

*are also bounded. Moreover, we have*

$$e^{itH} B(f) e^{-itH} \psi = B\left(e^{it(M-\tau M\tau)} f\right) \psi \quad , \qquad \forall\ \psi \in U_w^* F_+ \ , \tag{3.113}$$

*the exponential $e^{it(M-\tau M \tau)} f$ being defined in the sense of the power series.*

*Proof:* We first prove the claimed properties of $C$ and $M$ and relation (3.112). By hypothesis, $\tilde{H}$ can be represented as

$$\tilde{H} = \sum_{k,k' \in K} \left[ f_k \,\middle|\, \tilde{M} f_{k'} \right] B(f_k) B^*(f_{k'}) \ , \quad \text{with} \qquad \tilde{M} = w M w^{[*]} = \begin{pmatrix} c & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix} \ . \tag{3.114}$$

Since $\tau w \tau = w$, it follows that

$$w(M - \tau M \tau) w^{[*]} = \begin{pmatrix} c & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix} - \tau \begin{pmatrix} c & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix} \tau = C \ , \tag{3.115}$$

and hence (3.112) holds. Obviously $C$ is bounded. Since $w$ and $w^{[*]}$ are also bounded, so is

$$M - \tau M \tau = w^{[*]} C w \ . \tag{3.116}$$

We now prove relation (3.113) in the special case $H = \tilde{H}$, or, equivalently, $w = \mathbf{1}$. Obviously, it suffices to consider the case $\psi^{(n)} \in \mathcal{H}_+^n$, for some $n \in \mathbb{N}$, because we can then extend the relation by linearity to all finite vectors. First note that we have

$$H^k B(f) \psi^{(n)} = \sum_{l=0}^{k} \binom{k}{l} B(C^l f) H^{k-l} \psi^{(n)} \ . \tag{3.117}$$

This relation can easily be verified by an induction argument given in Lemma D.2. Secondly, we note that $H$ leaves invariant $\mathcal{H}_+^m$ and that $H\restriction_{\mathcal{H}_+^m}$ is an element of $\mathcal{B}(\mathcal{H}_+^m)$, for all $m \in \mathbb{N}$, since $H = \mathrm{d}\mathbf{G}(c)$ and $c \in \mathcal{B}(\mathcal{H}^1)$. Therefore, we have

$$\left\| H^k \psi^{(n)} \right\| \leq q^k \left\| \psi^{(n)} \right\| \qquad \text{with} \qquad q := \left\| H\restriction_{\mathcal{H}_+^n} \right\| \ , \tag{3.118}$$

for all $k \in \mathbb{N}$. By Stone's Theorem (see Lemma D.1), we have

$$e^{itH} B(f) \psi^{(n)} = \lim_{K \to \infty} \sum_{k=0}^{K} \frac{(it)^k}{k!} H^k B(f) \psi^{(n)} \tag{3.119}$$

and by (3.117), we have

$$\sum_{k=0}^{K} \frac{(it)^k}{k!} H^k B(f)\psi^{(n)} = \sum_{k=0}^{K} \frac{(it)^k}{k!} \sum_{l=0}^{k} \binom{k}{l} B(C^l f) H^{k-l} \psi^{(n)}$$
$$= \sum_{k=0}^{K} \sum_{l=0}^{k} \frac{(it)^l}{l!} B(C^l f) \frac{(it)^{k-l}}{(k-l)!} H^{k-l} \psi^{(n)} \ . \qquad (3.120)$$

We now show that the sums on the very right hand side of this relation can, in the limit $K \to \infty$, be decoupled in a manner similar to the Cauchy Product Formula. Namely, we have

$$\begin{aligned}
\text{l. h. s.} := & \left\| \sum_{k=0}^{K} \sum_{l=0}^{k} \frac{(it)^l}{l!} B(C^l f) \frac{(it)^{k-l}}{(k-l)!} H^{k-l} \psi^{(n)} \right. \\
& \qquad \left. - \sum_{l=0}^{K} \frac{(it)^l}{l!} B(C^l f) \sum_{k=0}^{K} \frac{(it)^k}{k!} H^k \psi^{(n)} \right\| \\
\leq & \sum_{\substack{k+l>K \\ 0\leq k,l\leq K}} \left\| \frac{(it)^l}{l!} B(C^l f)\restriction_{\mathcal{H}_+^n} \right\| \cdot \left\| \frac{(it)^k}{k!} H^k \psi^{(n)} \right\| \\
\leq & \sum_{\frac{K}{2}<l\leq K} \left\| \frac{(it)^l}{l!} B(C^l f)\restriction_{\mathcal{H}_+^n} \right\| \cdot \sum_{k=0}^{K} \left\| \frac{(it)^k}{k!} H^k \psi^{(n)} \right\| \\
& \qquad + \sum_{l=0}^{K} \left\| \frac{(it)^l}{l!} B(C^l f)\restriction_{\mathcal{H}_+^n} \right\| \cdot \sum_{\frac{K}{2}<k\leq K} \left\| \frac{(it)^k}{k!} H^k \psi^{(n)} \right\|
\end{aligned} \qquad (3.121)$$

Since, by Theorem 1.3,

$$\left\| B(C^l f)\restriction_{\mathcal{H}_+^n} \right\| \leq 2\sqrt{n+1}\, \| C \|^l \, \| f \| \quad , \qquad \forall\, l, n \in \mathbb{N} \ , \qquad (3.122)$$

and by (3.118) we can estimate further:

$$\text{l. h. s.} \ \leq \ 2\sqrt{n+1}\, \| f \| \left\| \psi^{(n)} \right\| \left( e^{tq} \sum_{l>\frac{K}{2}} \frac{t^l}{l!} \| C \|^l + e^{t\| C \|} \sum_{k>\frac{K}{2}} \frac{t^k}{k!} q^k \right) . \qquad (3.123)$$

Obviously, the right hand side of this inequality converges to zero as $K \to \infty$. Hence, (3.120) implies

$$\begin{aligned}
e^{itH} B(f)\psi^{(n)} &= \lim_{K\to\infty} \sum_{k=0}^{K} \frac{(it)^l}{l!} B(C^l f) \sum_{k=0}^{K} \frac{(it)^k}{k!} H^k \psi^{(n)} \\
&= \lim_{L\to\infty} \lim_{K\to\infty} \sum_{l=0}^{L} \frac{(it)^l}{l!} B(C^l f) \sum_{k=0}^{K} \frac{(it)^k}{k!} H^k \psi^{(n)} \\
&= \lim_{L\to\infty} \sum_{l=0}^{L} \frac{(it)^l}{l!} B(C^l f) e^{itH} \psi^{(n)} = B(e^{itC} f) e^{itH} \psi^{(n)} \ .
\end{aligned} \qquad (3.124)$$

In the last step we have used the fact that the mapping $f \in \mathcal{H}^1 \mapsto B(f)\lceil_{\mathcal{H}_+^n}$ is continuous by Theorem 1.2.

We have thus proved the theorem in the special case $w = \mathbf{1}$. As for the general case, we remark:

$$\begin{aligned} e^{itH}B(f)e^{-itH} &= U_w^* e^{it\tilde{H}} U_w B(f) U_w^* e^{-it\tilde{H}} U_w = U_w^* e^{it\tilde{H}} B(wf) e^{-it\tilde{H}} U_w \\ &= U_w^* B(e^{itC} wf) U_w = B(w^{[*]} e^{itC} wf) = B(e^{itw^{[*]}Cw} f) \ . \end{aligned} \tag{3.125}$$

We are done, since $w^{[*]}Cw = M - \tau M \tau$. □

### 3.1.4 The Generating Functional

This subsection is dedicated to the derivation of the generating functional $\mathcal{G}_H$ of a suitable quadratic operator $H$.

$$\mathcal{G}_H(g) := \frac{\operatorname{tr}\left(e^{i\Phi(g)} P\, e^{-H}\right)}{\operatorname{tr}\left(P\, e^{-H}\right)} \quad , \qquad \forall\, g \in \mathcal{H}^1 \ . \tag{3.126}$$

Here, $P$ is an orthogonal projection in $\mathcal{F}_+$ depending on the choice of $H$. (See Theorems 3.22 and 3.23 below.)

To this end, we introduce an over-complete family of vectors in $\mathcal{F}_+$, commonly known as bosonic coherent states. This family of states allows a decomposition of the identity, which we shall use to compute the values of the generating functional. For any $f \in \mathcal{H}^1$, we define the associated coherent state $\xi_f$ by

$$\xi_f \ := \ e^{i\left(a^*(f) + a(f)\right)} \Omega \ . \tag{3.127}$$

Note that the expression in the exponent of $e$ is a selfadjoint field, and thus we can make sense of this definition by the spectral theorem. Alternatively, we could also define the coherent states by

$$\xi_f = e^{-\frac{1}{2}\| f \|^2} \sum_{k=0}^{\infty} \frac{1}{\sqrt{k!}} f^{\otimes k} \ , \tag{3.128}$$

where the term corresponding to $k = 0$ is the vacuum. Moreover, it is possible to express the coherent state $\xi_f$ in terms of the following orthonormal basis in $\mathcal{F}_+$

$$\psi_{\underline{n}} := \sqrt{|\,\underline{n}\,|!}\ \mathcal{S}_+ \bigotimes_{j \in J} \left( \frac{1}{\sqrt{n_j!}} f_j^{\otimes n_j} \right) \qquad \text{and} \qquad \psi_{\underline{0}} := \Omega \ , \tag{3.129}$$

labeled by the occupation numbers

$$\underline{n} \in \mathbb{N}_0^J \ , \qquad \text{with} \qquad |\,\underline{n}\,| := \sum_{j \in J} n_j < \infty \ , \tag{3.130}$$

or, equivalently,

$$\psi_{\underline{n}} = \frac{1}{\sqrt{n_1! n_2! \cdots}} \big(a^*(f_1)\big)^{n_1} \big(a^*(f_2)\big)^{n_2} \cdots \Omega \ . \tag{3.131}$$

Here, $\{f_j\}_{j\in J}$ is an arbitrary orthonormal basis in $\mathcal{H}^1$. Without loss of generality, we set $J=\mathbb{N}$. We point out that tensor factors of the type $f^{\otimes 0}$ are understood to be absent, and operators of the type $\big(a^*(f_j)\big)^0$ are defined to be $\mathbf{1}$, such that in (3.129) only finite tensor products occur. To any $\underline{\alpha}\in\mathbb{C}^J$, with only finite $\alpha_j$'s different from zero, we associate

$$f_{\underline{\alpha}} := \sum_{j\in J}\alpha_j f_j \tag{3.132}$$

and may thus rewrite (3.128) to obtain

$$\xi_{f_{\underline{\alpha}}} = e^{-\frac{1}{2}\|\,\underline{\alpha}\,\|^2}\sum_{\underline{n}\in\mathbb{N}_0^J}\prod_{j\in J}\frac{\alpha_j^{n_j}}{\sqrt{n_j!}}\cdot\psi_{\underline{n}}\ . \tag{3.133}$$

*Proof of (3.133):* Let $f_{\underline{\alpha}}$ be as in (3.132) and set $J_{\underline{\alpha}} := \{j\in J \mid \alpha_j\neq 0\}$. It then holds true by (3.128):

$$\begin{aligned}
\xi_{f_{\underline{\alpha}}} &= e^{-\frac{1}{2}\|\,\underline{\alpha}\,\|^2}\sum_{n=0}^{\infty}\frac{1}{\sqrt{n!}}\Bigg(\sum_{j\in J_{\underline{\alpha}}}\alpha_j f_j\Bigg)^{\otimes n}\\
&= e^{-\frac{1}{2}\|\,\underline{\alpha}\,\|^2}\sum_{n=0}^{\infty}\frac{1}{\sqrt{n!}}\sum_{j:M_n\to J_{\underline{\alpha}}}\alpha_{j(1)}\cdots\alpha_{j(n)}\,f_{j(1)}\otimes\cdots\otimes f_{j(n)}\\
&= e^{-\frac{1}{2}\|\,\underline{\alpha}\,\|^2}\sum_{n=0}^{\infty}\frac{1}{\sqrt{n!}}\sum_{j:M_n\to J_{\underline{\alpha}}}\alpha_{j(1)}\cdots\alpha_{j(n)}\,\mathcal{S}_+ f_{j(1)}\otimes\cdots\otimes f_{j(n)}\ ,
\end{aligned}$$

where we have denoted $M_n := \{1,\ldots,n\}$, for all $n\in\mathbb{N}$. Again, the term corresponding to $n=0$ is defined to be the vacuum. We have made use of the fact that the sum over the mapping $j$ is invariant under the action of $\mathcal{S}_+$. After having interchanged the summation with this projection, we observe that the terms of the sum just depend on the cardinalities of the preimages of $j: M_n\to J_{\underline{\alpha}}$. Hence, we can rewrite the sum by the multinomial theorem to obtain

$$\xi_{f_{\underline{\alpha}}} = e^{-\frac{1}{2}\|\,\underline{\alpha}\,\|^2}\sum_{n=0}^{\infty}\sqrt{n!}\sum_{\underline{n}\,:\,|\,\underline{n}\,|=n}\mathcal{S}_+\bigotimes_{j\in J_{\underline{\alpha}}}\frac{\alpha_j^{n_j}}{n_j!}f_j^{\otimes n_j}\ . \tag{3.134}$$

From this and from the definition of $\psi_{\underline{n}}$, (3.133) follows. □

By the closedness of $a(g)$, for all $g\in\mathcal{H}^1$, we obtain:

$$a(g)\xi_f = \langle g\,|\,f\,\rangle\,\xi_f \qquad\text{and}\qquad e^{a(g)}\xi_f = e^{\langle g|\,f\,\rangle}\xi_f\ . \tag{3.135}$$

The left hand side of the second expression is defined in terms of the strongly convergent power-series. Furthermore, we have for an arbitrary, selfadjoint and nonnegative one-particle operator $h$ in $\mathcal{H}^1$:

$$e^{-\,\mathrm{d}\mathbf{G}(h)}\xi_f = e^{\frac{1}{2}\left\langle f\,\middle|\,(e^{-2h}-\mathbf{1})f\right\rangle}\xi_{e^{-h}f}\ . \tag{3.136}$$

This last formula follows from the observation $e^{-\,\mathrm{d}\mathbf{G}(h)} = \Gamma(e^{-h})$. A proof of this last observation may be found, e. g., in [31]. Moreover, we have

$$\mathbf{G}(Q)\xi_f = e^{-\frac{1}{2}\|\,Q^\perp f\,\|^2}\,\xi_{Qf}\ , \tag{3.137}$$

for any orthogonal projection $Q$ in $\mathcal{H}^1$ and arbitrary $f \in \mathcal{H}^1$. We now proceed, as announced, to prove a decomposition of the identity in terms of coherent states.

**Theorem 3.21.** *For any $\psi, \psi' \in \mathcal{F}_+$, we have, using notation* (3.132)*,*

$$\lim_{N\to\infty} \int \prod_{j=1}^{N} \frac{d\alpha_j\, d\bar{\alpha}_j}{\pi}\ \langle \psi \,|\, \xi_{f_{\underline{\alpha}}} \rangle\, \langle \xi_{f_{\underline{\alpha}}} \,|\, \psi' \rangle = \langle \psi \,|\, \psi' \rangle\ \ , \tag{3.138}$$

*where the $\alpha_j$'s with $j > N$ are set to zero.*

*Proof:* We use the following well-known fact about complex Gaussian integrals:

$$\int d\alpha\, d\bar{\alpha}\, \alpha^r \bar{\alpha}^{r'} e^{-|\,\alpha\,|^2} = \pi \cdot r! \cdot \delta_{r,r'} \quad , \qquad \forall\ r, r' \in \mathbb{N}_0\ . \tag{3.139}$$

To prove the theorem, we remark that, for any $N \in \mathbb{N}$,

$$\begin{aligned}
&\int \prod_{j=1}^{N} \frac{d\alpha_j\, d\bar{\alpha}_j}{\pi}\ \langle \psi \,|\, \xi_{f_{\underline{\alpha}}} \rangle\, \langle \xi_{f_{\underline{\alpha}}} \,|\, \psi' \rangle \\
&\quad = \int \prod_{j=1}^{N} \frac{d\alpha_j\, d\bar{\alpha}_j}{\pi} \sum_{\underline{m},\underline{n}\in\mathbb{N}^N} e^{-\|\,\underline{\alpha}\,\|^2} \prod_{j=1}^{N} \frac{\alpha_j^{m_j}\, \bar{\alpha}_j^{n_j}}{\sqrt{m_j! n_j!}}\, \langle \psi \,|\, \psi_{\underline{m}} \rangle\, \langle \psi_{\underline{n}} \,|\, \psi' \rangle \\
&\quad = \sum_{\underline{m},\underline{n}\in\mathbb{N}^N} \langle \psi \,|\, \psi_{\underline{m}} \rangle\, \langle \psi_{\underline{n}} \,|\, \psi' \rangle \prod_{j=1}^{N} \left[ \frac{1}{\sqrt{m_j! n_j!}} \int \frac{d\alpha\, d\bar{\alpha}}{\pi}\ \alpha^{m_j} \bar{\alpha}^{n_j} e^{-|\,\alpha\,|^2} \right] \\
&\quad = \sum_{\underline{n}\in\mathbb{N}^N} \langle \psi \,|\, \psi_{\underline{n}} \rangle\, \langle \psi_{\underline{n}} \,|\, \psi' \rangle \ \xrightarrow{N\to\infty}\ \langle \psi \,|\, \psi' \rangle\ \ .
\end{aligned} \tag{3.140}$$

Note that we have interchanged the summations over $\underline{m}$ and $\underline{n}$ with the integrals. This is a somewhat delicate point. For a proof of this, we refer the reader to [16, Sec. 1.6]. □

We are now in the position to formulate our main theorem concerning the generating functional. We proceed along the same lines as in Subsections 3.1.2 and 3.1.3, respectively, by proving the case of conserved number of particles first and generalizing later.

**Theorem 3.22.** *Let a selfadjoint one-particle operator $h$ in $\mathcal{H}^1$ be given such that $P^\perp_{\mathrm{kern}\,h} h P^\perp_{\mathrm{kern}\,h} \geq \varepsilon \cdot \mathbf{1} > 0$ and set $P := \mathbf{G}\left(P^\perp_{\mathrm{kern}\,h}\right)$. Furthermore, let*

$$P^\perp_{\mathrm{kern}\,h} \frac{e^{-h}}{\mathbf{1} - e^{-h}} P^\perp_{\mathrm{kern}\,h} \tag{3.141}$$

*be a trace-class operator. Then the generating functional*

$$\mathcal{G}_H(g) = \frac{\mathrm{tr}\left(e^{i\Phi(g)} P\, e^{-H}\right)}{\mathrm{tr}\left(P\, e^{-H}\right)} \tag{3.142}$$

*is well-defined, for all $g \in \mathcal{H}^1$, and has the following values:*

$$\mathcal{G}_{\mathrm{d}\mathbf{G}(h)}(g) = e^{-\frac{1}{4}\|\, g\,\|^2 - \frac{1}{2}\left\| \sqrt{e^{-h}(\mathbf{1}-e^{-h})^{-1}} P^{\perp}_{\mathrm{kern}\, h} g \right\|^2} . \tag{3.143}$$

*Proof:* We may assume that we are given an orthonormal basis $\{f_j\}_{j\in J}$ of eigenvectors of $h$. (This follows from the above trace-class assumption.) To each vector $f_j$, denote by $\lambda_j$ the associated eigenvalue. For any $g \in \mathcal{H}^1$, we show that

$$\mathrm{tr}\left(e^{i\Phi(g)} P e^{-\,\mathrm{d}\mathbf{G}(h)}\right) \tag{3.144}$$

is well-defined, and we determine its value. By relations (B.6) and (B.7), we have that

$$e^{i\Phi(g)}\psi = e^{-\frac{1}{4}\|\, g\,\|^2} e^{\frac{i}{\sqrt{2}}a^*(g)} e^{\frac{i}{\sqrt{2}}a(g)}\psi \quad , \qquad \forall\, \psi \in F_+ \,. \tag{3.145}$$

The operators $e^{\pm i a^*(g)}$ and $e^{\pm i a(g)}$ are defined in terms of their power-series in the strong operator topology. In particular, their domains contain the set of finite vectors. Note that, for any $\psi \in F_+$ and all $g \in \mathcal{H}^1$, $e^{\pm i a(g)}\psi$ is also a finite vector. Hence, the right hand side of (3.145) is well-defined. Moreover, for any $g \in \mathcal{H}^1$, we have

$$\begin{aligned}\left\langle \phi \,\middle|\, e^{\pm i a(g)}\psi \right\rangle &= \sum_{k=0}^{\infty} \left\langle \phi \,\middle|\, \frac{(\pm i)^k}{k!} a(g)^k \psi \right\rangle \\ &= \sum_{k=0}^{\infty} \left\langle \frac{(\mp i)^k}{k!} a^*(g)^k \phi \,\middle|\, \psi \right\rangle = \left\langle e^{\mp i a^*(g)}\phi \,\middle|\, \psi \right\rangle \ ,\end{aligned} \tag{3.146}$$

for all $\phi$ in the domain of $e^{\pm i a^*(g)}$ and all $\psi$ in the domain of $e^{\pm i a(g)}$ (and in particular for all finite $\psi, \phi \in F_+$). Relation (3.145) motivates us to consider first

$$\sum_{\underline{n}\in\mathbb{N}_0^J} \left\langle \psi_{\underline{n}} \,\middle|\, e^{i a^*(g)} e^{i a(g)} P e^{-\,\mathrm{d}\mathbf{G}(h)} \psi_{\underline{n}} \right\rangle \,. \tag{3.147}$$

Note that $Pe^{-\,\mathrm{d}\mathbf{G}(h)}$ leaves invariant the set of finite vectors. Therefore, all the above expectation values are well-defined. The following calculation serves two purposes: (i) In the special case $g = 0$, it will show that the above series of positive terms is finite, implying that $Pe^{-\,\mathrm{d}\mathbf{G}(h)}$ is trace-class. This will prove that (3.144) is well-defined. (ii) Once we know that (3.144) is well-defined, the same calculation, with $g \neq 0$, will help us to determine the value of the generating functional.

We have

$$
\begin{aligned}
\text{l. h. s.} :=& \sum_{\underline{n}\in\mathbb{N}_0^J} \left\langle \psi_{\underline{n}} \,\middle|\, e^{ia^*(g)} e^{ia(g)} P e^{-\,\mathrm{d}\mathbf{G}(h)} \psi_{\underline{n}} \right\rangle \\
=& \sum_{\underline{n}\in\mathbb{N}_0^J} \left\langle P e^{-\,\mathrm{d}\mathbf{G}(h/2)} e^{-ia^*(g)} e^{-ia(g)} \psi_{\underline{n}} \,\middle|\, P e^{-\,\mathrm{d}\mathbf{G}(h/2)} \psi_{\underline{n}} \right\rangle \\
=& \sum_{\underline{n}\in\mathbb{N}_0^J} \lim_{N\to\infty} \int \prod_{j=1}^{N} \frac{d\alpha_j\, d\bar{\alpha}_j}{\pi} \left\langle e^{-\,\mathrm{d}\mathbf{G}(h/2)} e^{-ia^*(g)} e^{-ia(g)} \psi_{\underline{n}} \,\middle|\, P \xi_{f_{\underline{\alpha}}} \right\rangle \\
& \qquad \left\langle P\xi_{f_{\underline{\alpha}}} \,\middle|\, e^{-\,\mathrm{d}\mathbf{G}(h/2)} \psi_{\underline{n}} \right\rangle \\
=& \sum_{\underline{n}\in\mathbb{N}_0^J} \lim_{N\to\infty} \int \prod_{j=1}^{N} \frac{d\alpha_j\, d\bar{\alpha}_j}{\pi} \left\langle e^{-\,\mathrm{d}\mathbf{G}(h/2)} e^{-ia^*(g)} e^{-ia(g)} \psi_{\underline{n}} \,\middle|\, \xi_{P^\perp_{\mathrm{kern}\,h} f_{\underline{\alpha}}} \right\rangle \\
& \qquad \left\langle \xi_{P^\perp_{\mathrm{kern}\,h} f_{\underline{\alpha}}} \,\middle|\, e^{-\,\mathrm{d}\mathbf{G}(h/2)} \psi_{\underline{n}} \right\rangle e^{-\| P_{\mathrm{kern}\,h} f_{\underline{\alpha}} \|^2} \;, \qquad (3.148)
\end{aligned}
$$

where we have used (3.146), (3.138) and (3.137). Let us collect the $j$'s such that $f_j$ is not in the kernel of $h$ in the sets

$$
J' := \{ j \in J \mid \lambda_j > 0 \} \qquad \text{and} \qquad J'_N := J' \cap \{1, \ldots, N\} \;, \qquad (3.149)
$$

for all $N \in \mathbb{N}$. The integrals over those $\alpha_j$'s with $j$ not in $J'$ may now be carried out, contributing a factor 1 each. We obtain:

$$
\begin{aligned}
\text{l. h. s.} =& \sum_{\underline{n}\in\mathbb{N}_0^J} \lim_{N\to\infty} \int \prod_{j\in J'_N} \frac{d\alpha_j\, d\bar{\alpha}_j}{\pi}\, e^{\langle f_{\underline{\alpha}} |\, (e^{-h} - \mathbf{1}) f_{\underline{\alpha}} \rangle}\, e^{i\langle g |\, e^{-h/2} f_{\underline{\alpha}} \rangle} \\
& \qquad \left\langle e^{-ia(g)} \psi_{\underline{n}} \,\middle|\, \xi_{e^{-h/2} f_{\underline{\alpha}}} \right\rangle \left\langle \xi_{e^{-h/2} f_{\underline{\alpha}}} \,\middle|\, \psi_{\underline{n}} \right\rangle \;, \qquad (3.150)
\end{aligned}
$$

where we have used relations (3.136), (3.146) and (3.135). We proceed by noting that

$$
e^{-ia(g)} \psi_{\underline{n}} = \sum_{\underline{k}\in\mathbb{N}_0^J,\; \underline{k}\le\underline{n}} \prod_{j\in J} \left[ \frac{(-i\bar{\beta}_j)^{k_j}}{k_j!} \sqrt{\frac{n_j!}{(n_j - k_j)!}} \right] \psi_{\underline{n}-\underline{k}} \;, \qquad (3.151)
$$

for $g = \sum_{j\in\mathbb{N}} \beta_j f_j \in \mathcal{H}^1$ and all finite occupation numbers $\underline{n}$. By $\underline{k} \le \underline{n}$, we mean $k_j \le n_j$, for all $j \in J$. (3.151) follows directly from the definition of the left hand side of (3.151) as a power-series. Furthermore, we have by relation (3.133)

$$
\left\langle \psi_{\underline{n}} \,\middle|\, \xi_{e^{-h/2} f_{\underline{\alpha}}} \right\rangle = \prod_{j\in J} \left[ e^{-\frac{1}{2}\varepsilon_j^2 |\alpha_j|^2} \frac{\varepsilon_j^{n_j} \alpha_j^{n_j}}{\sqrt{n_j!}} \right] \;, \qquad (3.152)
$$

where we have set $\varepsilon_j := e^{-\frac{1}{2}\lambda_j}$, for all $j \in J$. Note that this expression evaluates to zero, if $n_j > 0$, for some $j$ such that $\alpha_j = 0$. Combining (3.151) with (3.152), we obtain

$$
\begin{aligned}
\left\langle e^{-ia(g)} \psi_{\underline{n}} \,\middle|\, \xi_{e^{-h/2} f_{\underline{\alpha}}} \right\rangle =& \sum_{\underline{k}\in\mathbb{N}_0^J,\; \underline{k}\le\underline{n}} \prod_{j\in J} \left[ \frac{(i\beta_j)^{k_j}}{k_j!} \sqrt{\frac{n_j!}{(n_j - k_j)!}} \right] \\
& \qquad \prod_{j\in J} \left[ e^{-\frac{1}{2}\varepsilon_j^2 |\alpha_j|^2} \frac{\varepsilon_j^{n_j - k_j} \alpha_j^{n_j - k_j}}{\sqrt{(n_j - k_j)!}} \right] \;. \qquad (3.153)
\end{aligned}
$$

We now insert (3.152) and (3.153) into (3.150). This yields

$$
\begin{aligned}
\text{l. h. s.} = & \sum_{\underline{n}\in\mathbb{N}_0^J} \lim_{N\to\infty} \int \prod_{j\in J'_N} \frac{d\alpha_j\, d\bar{\alpha}_j}{\pi}\, e^{\sum_{j\in J'_N} (\varepsilon_j^2-1)|\,\alpha_j\,|^2}\, e^{i\sum_{j\in J'_N} \bar{\beta}_j\varepsilon_j\alpha_j} \\
& \sum_{\underline{k}\in\mathbb{N}_0^{J'},\ \underline{k}\le\underline{n}} \prod_{j\in J} \left[ \frac{(i\beta_j)^{k_j}}{k_j!} \sqrt{\frac{n_j!}{(n_j-k_j)!}} \right] \prod_{j\in J} \left[ e^{-\frac{1}{2}\varepsilon_j^2|\,\alpha_j\,|^2} \frac{\varepsilon_j^{n_j-k_j}\alpha_j^{n_j-k_j}}{\sqrt{(n_j-k_j)!}} \right] \\
& \prod_{j\in J} \left[ e^{-\frac{1}{2}\varepsilon_j^2|\,\alpha_j\,|^2} \frac{\varepsilon_j^{n_j}\bar{\alpha}_j^{n_j}}{\sqrt{n_j!}} \right] \\
= & \sum_{\underline{n}\in\mathbb{N}_0^J} \lim_{N\to\infty} \int \prod_{j\in J'_N} \frac{d\alpha_j\, d\bar{\alpha}_j}{\pi}\, e^{\sum_{j\in J'_N}|\,\alpha_j\,|^2} \\
& \prod_{j\in J'_N} \left[ \varepsilon_j^{n_j}\bar{\alpha}_j^{n_j} \sum_{r=0}^{\infty}\sum_{k=0}^{n_j} \frac{1}{r!k!(n_j-k)!} (i\beta_j\varepsilon_j\alpha_j)^r (i\beta_j)^k (\varepsilon_j\alpha_j)^{n_j-k} \right] ,
\end{aligned}
\tag{3.154}
$$

where we have used the fact that the integral evaluates to zero if $n_j \neq 0$, for some $j$ not in $J'_N$. We now factorize the integration, and obtain the following expression involving the infinite product $\prod_{j\in J'}$:

$$
\begin{aligned}
\text{l. h. s.} = & \sum_{\underline{n}\in\mathbb{N}_0^J} \prod_{j\in J'} \int \frac{d\alpha\, d\bar{\alpha}}{\pi}\, e^{-|\,\alpha\,|^2} \\
& \left[ \varepsilon_j^{n_j}\bar{\alpha}^{n_j} \sum_{r=0}^{\infty}\sum_{k=0}^{n_j} \frac{1}{r!k!(n_j-k)!} (i\beta_j\varepsilon_j\alpha)^r (i\beta_j)^k (\varepsilon_j\alpha)^{n_j-k} \right] .
\end{aligned}
\tag{3.155}
$$

Note that only the terms with $k = r$ contribute to the integral due to relation (3.139). Therefore, we have

$$
\begin{aligned}
\text{l. h. s.} &= \sum_{\underline{n}\in\mathbb{N}_0^J} \prod_{j\in J'} \int \frac{d\alpha\, d\bar{\alpha}}{\pi}\, e^{-|\,\alpha\,|^2} \left[ \varepsilon_j^{2n_j} |\,\alpha\,|^{2n_j} \sum_{k=0}^{n_j} \frac{1}{(k!)^2(n_j-k)!} (-|\,\beta_j\,|^2)^k \right] \\
&= \sum_{\underline{n}\in\mathbb{N}_0^J} \prod_{j\in J'} \left[ \varepsilon_j^{2n_j} \sum_{k=0}^{n_j} \frac{n_j!}{(k!)^2(n_j-k)!} (-|\,\beta_j\,|^2)^k \right] \\
&= \prod_{j\in J'} \left[ \sum_{n=0}^{\infty} \varepsilon_j^{2n} \sum_{k=0}^{n} \frac{n!}{(k!)^2(n-k)!} (-|\,\beta_j\,|^2)^k \right] \\
&= \prod_{j\in J'} \left[ \sum_{k=0}^{\infty} \frac{1}{k!} (-|\,\beta_j\,|^2)^k \varepsilon_j^{2k} \sum_{n=0}^{\infty} \frac{(n+k)!}{k!n!} \varepsilon_j^{2n} \right] .
\end{aligned}
\tag{3.156}
$$

The factoring out we have performed, schematically $\sum_{\underline{n}}\prod_j \cdots = \prod_j \sum_n \ldots$, is obtained by iterated application of the Cauchy product formula (note that all appearing factors are positive). Furthermore we have used the summation formula $\sum_{n=0}^{\infty}\sum_{r=0}^{n} q_{n,r} = \sum_{n=0}^{\infty}\sum_{r=0}^{\infty} q_{n+r,r}$. Let us now remark that the inner summation corresponds to a binomial series with negative exponent $-k-1$ and so we obtain:

$$\text{l. h. s.} = \prod_{j\in J'}\left[\sum_{k=0}^{\infty}\frac{1}{k!}(-\mid\beta_j\mid^2)^k\varepsilon_j^{2k}\left(\frac{1}{1-\varepsilon_j^2}\right)^{k+1}\right]$$
$$= \prod_{j\in J'}\left[\frac{1}{1-\varepsilon_j^2}\exp\left(-\mid\beta_j\mid^2\frac{\varepsilon_j^2}{1-\varepsilon_j^2}\right)\right] , \quad (3.157)$$

where l. h. s. is given by (3.148). The infinite product on the right hand side exists by assumption. In particular, we note that for $g=0$, or, equivalently, $\beta_j=0$, for all $j\in J$, it follows that $e^{-\,\mathrm{d}\mathbf{G}(h)}$ is indeed trace-class by the trace-class assumption on (3.141). Hence, (3.144) is well-defined. Together with (3.145), we deduce:

$$\frac{\operatorname{tr}\left(e^{i\Phi(g)}Pe^{-\,\mathrm{d}\mathbf{G}(h)}\right)}{\operatorname{tr}\left(Pe^{-\,\mathrm{d}\mathbf{G}(h)}\right)} = \exp\left(-\frac{1}{4}\parallel g\parallel^2-\frac{1}{2}\left\|\sqrt{e^{-h}(\mathbf{1}-e^{-h})^{-1}}P^{\perp}_{\mathrm{kern}\,h}g\right\|^2\right) \quad (3.158)$$

completing our proof.

□

We now generalize to the case, where the number of particles is not necessarily conserved. To this end, let $\{f_k\}_{k\in K}$ be a self-dual basis in $\mathcal{K}$ such that $\{f_k\}_{k\in K_\pm}$ is an orthonormal basis in $\mathcal{K}_\pm$, respectively.

**Theorem 3.23.** *Let $H$ be a selfadjoint operator in $\mathcal{F}_+$. Suppose there exists a homogeneous Bogoliubov transformation $w$ of the form*

$$w=\begin{pmatrix} X & Y\\ \bar{Y} & \bar{X}\end{pmatrix} , \quad \textit{for some } X,Y\in\mathcal{B}(\mathcal{H}^1) , \quad (3.159)$$

*possessing a unitary implementation $U_w$ such that*

$$\tilde{H}:=U_wHU_w^*=\mathrm{d}\mathbf{G}(h) , \quad (3.160)$$

*for some selfadjoint one-particle operator $h$, complying with the hypothesis of Theorem 3.22. The generating functional for such an $H$ has the form*

$$\mathcal{G}_H(g)=\exp\left(-\frac{1}{4}\parallel\tilde{g}\parallel^2-\frac{1}{2}\left\|\sqrt{e^{-h}(\mathbf{1}-e^{-h})}P^{\perp}_{\mathrm{kern}\,h}\tilde{g}\right\|^2\right) , \quad (3.161)$$

*for $\tilde{g}:=Xg+\bar{Y}g$.*

*Proof:* Note that, since $U_w\Phi(g)U_w^*=\Phi(\tilde{g})$, we have $\mathcal{G}_H(g)=\mathcal{G}_{\tilde{H}}(\tilde{g})$. □

## 3.2 Fermionic Theory

### 3.2.1 Quasi-Free States

In the fermion case we define the property of a state being quasi-free directly in terms of the expectations of the monomials of the generators $B(\cdot)$ of the self-dual algebra. We recall that all the following considerations concern even states, only.

**Definition 3.24.** *An even state $\omega$ is called* <u>*quasi-free*</u> *if its hierarchy of truncated functionals $\omega^{(t)}$ satisfies:*

$$\omega^{(t)}(f_1, \ldots, f_n) = 0 \quad , \qquad \forall\, n \geq 3,\ f_1, \ldots, f_n \in \mathcal{L} \ . \tag{3.162}$$

Obviously we have, for any quasi-free state $\omega$, $\omega^{(t)}(f,g) = \omega\big(B(f)B(g)\big)$. Completely analogous to the boson case, it is possible to prove:

**Lemma 3.25.** *For any even state $\omega$, arbitrary $n \geq 3$ and all $f_1, \ldots, f_n \in \mathcal{L}$ it holds:*

$$\omega^{(t)}(f_{\pi(1)}, \ldots, f_{\pi(n)}) = \mathrm{sign}(\pi) \cdot \omega^{(t)}(f_1, \ldots, f_n) \quad , \qquad \forall\, \pi \in S_n \ . \tag{3.163}$$

*Proof:* Let us first point out that in the fermion case all odd elements of the hierarchy of truncated functionals of $\omega$ vanish identically, i. e.,

$$\omega^{(t)}(f_1, \ldots, f_{2n-1}) = 0 \quad , \qquad \forall\, f_1, \ldots, f_{2n-1} \in \mathcal{L} \ , \tag{3.164}$$

since we have assumed that $\omega$ itself is even. On solving equations (1.116) in the cases $n = 2, 4$, we obtain:

$$\begin{aligned} \omega^{(t)}(f_1, f_2, f_3, f_4) = {} & \omega\big(B(f_1)B(f_2)B(f_3)B(f_4)\big) \\ & - \omega\big(B(f_1)B(f_2)\big)\omega\big(B(f_3)B(f_4)\big) + \omega\big(B(f_1)B(f_3)\big)\omega\big(B(f_2)B(f_4)\big) \\ & - \omega\big(B(f_1)B(f_4)\big)\omega\big(B(f_2)B(f_3)\big) \ . \end{aligned} \tag{3.165}$$

By this relation and the CAR (1.86), it is easy to see that the claim is true for $n = 4$. With the aid of this observation and the fact that all odd $n$-point functions of $\omega$ vanish, the induction argument in the proof of Lemma 3.4 p. 37 carries over to the present situation, almost word by word. We merely need to insert at each step of the argument the sign of the corresponding partition. □

### 3.2.2 Generalized Density Matrices

In this subsection we basically translate some results in [8] into our notation, reproducing the proofs in a slightly modified form.

**Definition 3.26.** *An operator $\Gamma$ in $\mathcal{B}(\mathcal{L})$ obeying $\mathbf{0} \leq \Gamma \leq \mathbf{1}$ and of the form*

$$\Gamma = \begin{pmatrix} \gamma & \alpha \\ -\bar{\alpha} & \mathbf{1} - \bar{\gamma} \end{pmatrix} \tag{3.166}$$

*with respect to Decomposition (1.80) is called a* <u>*generalized density matrix*</u>*. The associated quadratic form*

$$\Gamma(f,g) := \langle f \,|\, \Gamma g \rangle \tag{3.167}$$

*is also called generalized density matrix.*

Note that (3.166) is equivalent to

$$\tau \Gamma \tau = \mathbf{1} - \Gamma \ . \tag{3.168}$$

This relation translates to the quadratic form as follows:

$$\Gamma(f,g) = \langle f \,|\, g\rangle - \Gamma(\tau g, \tau f) \quad , \qquad \forall\ f,g \in \mathcal{L}\ . \tag{3.169}$$

For any state $\omega$, we denote by $\Gamma_\omega$ the generalized density matrix given by

$$\Gamma_\omega(f,g) := \omega\big(B(g)B^*(f)\big) \quad , \qquad \forall\ f,g \in \mathcal{L}\ . \tag{3.170}$$

The definition of the conjugation $\tau$, the CAR and the positivity property of $\omega$ guarantee, that $\Gamma_\omega$ is indeed a generalized density matrix in the sense of Definition 3.26.

Furthermore, we can recover from $\Gamma$ by restriction to $\mathcal{L}_+$, what is called reduced density matrix[7] or just density matrix and denoted by $\gamma$:

$$\gamma := P_{\mathcal{L}_+} \Gamma P_{\mathcal{L}_+}\ . \tag{3.172}$$

For any state $\omega$, we thus have

$$\gamma_\omega(f,g) = \omega\big(a^*(g)a(f)\big) \quad , \qquad \forall\ f,g \in \mathcal{H}^1\ . \tag{3.173}$$

**Definition 3.27.** *A generalized density matrix $\Gamma$ is called an admissible generalized density matrix if and only if $\gamma := P_{\mathcal{L}_+}\Gamma P_{\mathcal{L}_+}$ is trace-class in the Hilbert space $\mathcal{L}_+$. In this case $\mathrm{tr}_{\mathcal{L}_+}(\gamma)$ is called the particle number of $\Gamma$. If, additionally*

$$P_{\mathcal{L}_+}\Gamma P_{\mathcal{L}_-} = P_{\mathcal{L}_-}\Gamma P_{\mathcal{L}_+} = \mathbf{0}\ , \tag{3.174}$$

*then $\Gamma$ is said to conserve particle number.*

**Definition 3.28.** *A state $\omega$ is called an admissible state if and only if $\Gamma_\omega$ is an admissible generalized density matrix and its one-point functional $f \mapsto \omega\big(a^*(f)\big)$ is continuous. If, additionally,*

$$\omega\big(a^*(f_1)\cdots a^*(f_n)a(g_1)\cdots a(g_m)\big) = 0\ , \tag{3.175}$$

*for all $f_1,\cdots,f_n,g_1,\dots,g_m \in \mathcal{H}^1$ and $m \neq n$, then $\omega$ is said to conserve particle number.*

For any fermionic generalized density matrix $\Gamma$, we have $\Gamma^2 \leq \Gamma$. If $\Gamma$ is admissible, we may infer from the upper left block (see (3.166)) of this inequality $\mathrm{tr}(\gamma^2)+\mathrm{tr}(\alpha^*\alpha) \leq \mathrm{tr}(\gamma) < \infty$ and thus $\alpha$ must be Hilbert-Schmidt, just as in the boson case.

Similarly to the boson case, if $\Gamma = \Gamma_\omega$, for some state $\omega$, then $\alpha$ and $\gamma$ are determined by

$$\langle f \,|\, \gamma g\rangle = \omega\big(a^*(g)a(f)\big) \qquad \text{and} \qquad \langle f \,|\, \alpha g\rangle = \omega\big(a(\bar g)a(f)\big) \quad , \qquad \forall\ f,g \in \mathcal{H}^1. \tag{3.176}$$

Obviously, the set of admissible generalized density matrices is convex.

We now show that $\omega \mapsto \Gamma_\omega$ maps the set of all admissible quasi-free states bijectively onto the admissible generalized density matrices. To this end, we first consider the case of conserved particle number.

[7] Also in this case, we shall draw no linguistic nor notational distinction between the operator $\gamma$ and the quadratic form

$$\gamma(f,g) := \langle f \,|\, \gamma g\rangle \quad , \qquad \forall\ f,g \in \mathcal{H}^1\ . \tag{3.171}$$

**Proposition 3.29.** *Let* $\Gamma$ *be an admissible generalized density matrix with conserved number of particles. Suppose* $\Gamma$ *obeys the additional condition* $\gamma \leq (1-\varepsilon)\cdot \mathbf{1}$*, for some* $\varepsilon > 0$*. Then there exists an admissible state* $\omega$ *with conserved particle number, given by*

$$\omega(\cdot) := \frac{\mathrm{tr}\left(\cdot\, Pe^{-\,\mathrm{d}\mathbf{G}(h)}\right)}{\mathrm{tr}\left(Pe^{-\,\mathrm{d}\mathbf{G}(h)}\right)}\ , \tag{3.177}$$

*with*

$$h = P^{\perp}_{\mathrm{kern}\,\gamma} \ln\left(\frac{1-\gamma}{\gamma}\right) P^{\perp}_{\mathrm{kern}\,\gamma} \qquad \textit{and} \qquad P := \mathbf{G}(P^{\perp}_{\mathrm{kern}\,\gamma}) \tag{3.178}$$

*having* $\Gamma$ *as its generalized density matrix.*

The condition on $\gamma$ in the hypothesis of this proposition excludes the possibility of $\gamma$ being a projection. See, however, Lemma 3.30.

*Proof of Proposition 3.29:* Let us first remark that $\gamma$, being trace-class, possesses a complete orthonormal set $\{f_j\}_{j\in\mathbb{N}}$ of eigenvectors and denote by $\gamma_j \in [0, 1-\varepsilon]$ the eigenvalue of $\gamma$ corresponding to $f_j$. By construction, an eigenvector $f_j$ of $\gamma$ is also an eigenvector of $h$ and we denote the corresponding eigenvalue by $\lambda_j$. We then have

$$\lambda_j = \begin{cases} \ln\left(\frac{1-\gamma_j}{\gamma_j}\right) & \text{if } 0 < \gamma_j \leq 1-\varepsilon \\ 0 & \text{if } \gamma_j = 0 \end{cases} . \tag{3.179}$$

We now show that $Pe^{-\,\mathrm{d}\mathbf{G}(h)}$ is trace-class, thus proving the well-definedness of $\omega$. To this end, denote

$$J' := \{\, j \in \mathbb{N} \mid \gamma_j > 0 \,\}\ . \tag{3.180}$$

We evaluate the trace of $Pe^{-\,\mathrm{d}\mathbf{G}(h)}$ in the orthonormal basis given by the vectors

$$\psi_{\underline{n}} := \big(a^*(f_1)\big)^{n_1}\big(a^*(f_2)\big)^{n_2}\cdots\Omega\ , \tag{3.181}$$

for all finite occupation numbers

$$\underline{n} \in \{0,1\}^{\mathbb{N}} \qquad \text{with} \qquad |\,\underline{n}\,| := \sum_{j\in\mathbb{N}} n_j < \infty\ . \tag{3.182}$$

By direct computation, we obtain:

$$\begin{aligned} \mathrm{tr}\left(Pe^{-\,\mathrm{d}\mathbf{G}(h)}\right) &= \sum_{\underline{n}\in\{0,1\}^{J'}} \prod_{j\in J'} e^{-\lambda_j n_j} = \prod_{j\in J'}(1+e^{-\lambda_j}) \\ &= \prod_{j\in J'}\left(1+\frac{\gamma_j}{1-\gamma_j}\right) = \prod_{j\in\mathbb{N}} \frac{1}{1-\gamma_j} < \infty\ . \end{aligned} \tag{3.183}$$

(Note that we could drop the restriction on $j$ in the last step). The convergence of the infinite product on the right hand side is implied by the trace-class property of $\gamma$, which is given by hypothesis. To see this, just take the logarithm of the partial product of the expression on the right hand side. (For a review on the theory of convergence of infinite products, see e. g. [33].)

It remains to prove that $\omega$ is in fact quasi-free and that it has $\Gamma$ as its generalized density matrix. With regard to the second point, we observe:

$$\begin{aligned}
&\omega\left(B\left(\begin{pmatrix} f_j \\ f_{j'} \end{pmatrix}\right)B^*\left(\begin{pmatrix} f_l \\ f_{l'} \end{pmatrix}\right)\right) \\
&= \frac{1}{\operatorname{tr}\left(Pe^{-\,\mathrm{d}\mathbf{G}(h)}\right)}\left(\delta_{j,l}\operatorname{tr}\left(a^*(f_j)a(f_l)Pe^{-\,\mathrm{d}\mathbf{G}(h)}\right)+\delta_{j',l'}\operatorname{tr}\left(a(\bar f_{j'})a^*(\bar f_{l'})Pe^{-\,\mathrm{d}\mathbf{G}(h)}\right)\right) \\
&= \frac{1}{\operatorname{tr}\left(Pe^{-\,\mathrm{d}\mathbf{G}(h)}\right)}\left(\delta_{j,l}\gamma_j\operatorname{tr}\left(Pe^{-\,\mathrm{d}\mathbf{G}(h)}\right)+\delta_{j',l'}(1-\gamma_{j'})\operatorname{tr}\left(Pe^{-\,\mathrm{d}\mathbf{G}(h)}\right)\right) \\
&= \delta_{j,l}\gamma_j+\delta_{j',l'}(1-\gamma_{j'}) = \Gamma\left(\begin{pmatrix} f_l \\ f_{l'} \end{pmatrix},\begin{pmatrix} f_j \\ f_{j'} \end{pmatrix}\right)\ ,
\end{aligned}$$

where we have concluded, similarly as in (3.183),

$$\begin{aligned}
\operatorname{tr}\left(a^*(f_l)a(f_l)Pe^{-\,\mathrm{d}\mathbf{G}(h)}\right) &= e^{-\lambda_l}\sum_{\underline{n}\in\{0,1\}^{J'\setminus\{l\}}}\ \prod_{j\in J'\setminus\{l\}}(1-e^{-\lambda_j}) \\
&= \frac{\gamma_l}{1-\gamma_l}\prod_{j\neq l}\frac{1}{1-\gamma_j} = \gamma_j\prod_j\frac{1}{1-\gamma_j} = \gamma_j\operatorname{tr}\left(Pe^{-\,\mathrm{d}\mathbf{G}(h)}\right)\ . \qquad (3.184)
\end{aligned}$$

For a proof of quasi-freeness we refer the reader to [8]. It is there shown that $\omega$ may be represented as a limit of Gibbs states, which are known to be quasi-free (see e. g. [17]). □

**Lemma 3.30.** *To any admissible generalized density matrix $\Gamma$, there exists a self-dual decomposition of $\mathcal{L}$ given by*

$$\mathcal{L} = \tilde{\mathcal{L}}_+ \oplus \tilde{\mathcal{L}}_- \qquad (3.185)$$

*into an orthogonal direct sum, such that the spaces $\tilde{\mathcal{L}}_\pm$ are invariant subspaces of $\Gamma$ and moreover*

$$\mathbf{0}\ \leq\ \Gamma\restriction_{\tilde{\mathcal{L}}_+}\ \leq\ \tfrac{1}{2}\cdot\mathbf{1}\ . \qquad (3.186)$$

*Proof:* The following simple argument, taken from [8], shows that $\Gamma$ possesses a complete orthonormal set of eigenvectors: Since $\Gamma(\mathbf{1}-\Gamma)$ is a selfadjoint trace-class operator, it does indeed possess a complete orthonormal set of eigenvectors $\{g_j\}_{j\in I}$. Denote the associated eigenvalues by $\{\mu_j\}_{j\in I}$. On the other hand, $\Gamma$ leaves invariant any of the following two dimensional subspaces

$$\operatorname{span}\{g_j,\Gamma g_j\}\ , \qquad (3.187)$$

for any $j$, since $\Gamma^2 g_j = -\Gamma(\mathbf{1}-\Gamma)g_j+\Gamma g_j = -\mu_j g_j+\Gamma g_j$. Since $\Gamma$ is symmetric, it possesses in turn a complete orthonormal set of eigenvectors.

Now, if $f$ is an eigenvector of $\Gamma$ associated to the eigenvalue $\lambda$, then by (3.168) we have

$$\Gamma\tau f = \tau(\mathbf{1}-\Gamma)f = (1-\lambda)\tau f \qquad (3.188)$$

and therefore $1-\lambda$ is also an eigenvalue of $\Gamma$ and $\tau f$ a corresponding eigenvector. We can thus divide the index set $I$ into two disjoint sets

$$I = I_+\ \dot\cup\ I_- \qquad (3.189)$$

of equal cardinality such that $0 \leq \mu_i \leq \frac{1}{2}$, for all $i \in I_+$. Setting

$$\tilde{\mathcal{L}}_\pm := \overline{\mathrm{span}\{f_i\}_{i\in I_\pm}} \;, \tag{3.190}$$

we have achieved our goal of constructing the invariant subspaces and obviously (3.186) is fulfilled. □

**Lemma 3.31.** *If $\Gamma$ is an admissible generalized density matrix and $w$ is a homogeneous Bogoliubov transformation, mapping the subspaces $\mathcal{L}_\pm$ unitarily onto the invariant subspaces $\tilde{\mathcal{L}}_\pm$ of $\Gamma$, and furthermore* (3.186) *holds, then the following defines an admissible generalized density matrix $\tilde{\Gamma}$:*

$$\tilde{\Gamma} := w^*\Gamma w \tag{3.191}$$

*Moreover, the transformation $w$ has a unitary implementation.*

*Proof:* Evidently $\tilde{\Gamma}$ is a generalized density matrix. In order to prove its admissibility we note: With respect to the decomposition (1.80), we may write

$$\Gamma = \begin{pmatrix} \gamma & \alpha \\ -\bar{\alpha} & \mathbf{1}-\bar{\gamma} \end{pmatrix} \qquad \text{and} \qquad \tilde{\Gamma} = \begin{pmatrix} \tilde{\gamma} & \mathbf{0} \\ \mathbf{0} & \mathbf{1}-\bar{\tilde{\gamma}} \end{pmatrix} \;, \tag{3.192}$$

for some operators $\tilde{\gamma}$, $\gamma$ and $\alpha$ in $\mathcal{H}^1$. By the properties of $\Gamma$, we have that $\gamma \geq 0$ is trace-class and that $\alpha^T = -\alpha$. Similar to the boson case, we have

$$\mathrm{tr}\left(\tilde{\Gamma}(\mathbf{1}-\tilde{\Gamma})\right) = \mathrm{tr}\left(\Gamma(\mathbf{1}-\Gamma)\right) \;. \tag{3.193}$$

Reexpressing this equality in terms of $\alpha$, $\gamma$ and $\tilde{\gamma}$, we obtain

$$\mathrm{tr}(\tilde{\gamma}) - \mathrm{tr}(\tilde{\gamma}^2) = \mathrm{tr}(\gamma) - \mathrm{tr}(\gamma^2) + \mathrm{tr}(\alpha^*\alpha) \;. \tag{3.194}$$

By the admissibility of $\Gamma$, the right hand side of this equation is finite. (We recall in particular that admissibility also implies the Hilbert-Schmidt condition for $\alpha$.) The left hand side may be estimated, since (3.186) is assumed, from below by $\frac{1}{2}\,\mathrm{tr}(\tilde{\gamma})$. This implies

$$\mathrm{tr}(\tilde{\gamma}) < \infty \tag{3.195}$$

and therefore $\tilde{\Gamma}$ is admissible. We shall now show that $w$ possesses a unitary implementation. To this end, we express $w$ as a $2\times 2$ block matrix with respect to the decomposition (1.80)

$$w = \begin{pmatrix} X & Y \\ \bar{Y} & \bar{X} \end{pmatrix} \;, \tag{3.196}$$

for suitable operators $X, Y \in \mathcal{B}(\mathcal{H}^1)$, obeying relations (2.12). We have by (3.191)

$$\tilde{\gamma} = X^*\gamma X + X^*\alpha\bar{Y} - Y^T\bar{\alpha}X + Y^T(1-\bar{\gamma})\bar{Y} \tag{3.197}$$

and hence

$$\infty > \mathrm{tr}\left(X^*\gamma X + X^*\alpha\bar{Y} - Y^T\bar{\alpha}X - Y^T\bar{\gamma}\bar{Y}\right) + \mathrm{tr}(Y^*Y) \;. \tag{3.198}$$

The first trace on the right hand side may be estimated as follows:

$$\begin{aligned} &\mathrm{tr}\left(X^*\gamma X + X^*\alpha\bar{Y} - Y^T\bar{\alpha}X - Y^T\bar{\gamma}\bar{Y}\right) \\ &\qquad \geq -\,\mathrm{tr}(XX^*\gamma) - 2\sqrt{\mathrm{tr}(Y^*Y)}\sqrt{\mathrm{tr}(XX^*\alpha\alpha^*)} - \mathrm{tr}(YY^*\gamma) \\ &\qquad\qquad = -\,\mathrm{tr}(\gamma) - 2\sqrt{\mathrm{tr}(Y^*Y)}\sqrt{\mathrm{tr}(XX^*\alpha\alpha^*)} \;, \end{aligned} \tag{3.199}$$

where in the last step we have used $\gamma \geq 0$ and $XX^* + YY^* = \mathbf{1}$. Combining the last two inequalities, we obtain

$$\begin{aligned}\infty > \mathrm{tr}(Y^*Y) - \mathrm{tr}(\gamma) - 2\sqrt{\mathrm{tr}(Y^*Y)}\sqrt{\mathrm{tr}(XX^*\alpha\alpha^*)} \\ = \Big(\sqrt{\mathrm{tr}(Y^*Y)} - \sqrt{\mathrm{tr}(XX^*\alpha\alpha^*)}\Big)^2 - \mathrm{tr}(XX^*\alpha\alpha^*) - \mathrm{tr}(\gamma)\ .\end{aligned} \tag{3.200}$$

By the fact that $\alpha$ is Hilbert-Schmidt, since $\gamma$ is trace-class and also by the boundedness of $X$, it follows that $\mathrm{tr}(YY^*) < \infty$, proving that $w$ possesses a unitary implementation. □

Proposition 3.29 together with Lemmas 3.30 and 3.31 proves:

**Theorem 3.32.** *If $\Gamma$ is an admissible generalized density matrix, then there is an admissible even quasi-free state $\omega$, having $\Gamma$ as its generalized density matrix.*

This shows that the admissible quasi-free states with vanishing one-point function are in 1:1-correspondence with the admissible generalized density matrices.

### 3.2.3 Quadratic Operators

In this subsection, we discuss selfadjoint operators in fermion Fock space $\mathcal{F}_-$, which can be expressed quadratically in the fermion particle annihilation and particle creation operators $a(\cdot)$ and $a^*(\cdot)$. Let $\{f_k\}_{k\in\mathbb{N}}$ be an orthonormal basis in $\mathcal{H}^1$. Namely, we consider operators of the form

$$H \ := \ \mathrm{d}\mathbf{G}(c) + \sum_{k,k'\in I} \big(b_{k,k'}a^*(f_k)a^*(\bar{f}_{k'}) + \bar{b}_{k,k'}a(\bar{f}_k)a(f_{k'})\big)\ , \tag{3.201}$$

for some selfadjoint operator $c$ in $\mathcal{H}^1$, some *finite* index set $I$ and arbitrary numbers $\{b_{k,k'}\}_{k,k'\in I}$ obeying $b_{k,k'} = -b_{k',k}$. $\mathrm{d}\mathbf{G}(c)$ is selfadjoint in $\mathcal{F}_-$ and the remaining terms are symmetric and bounded. Therefore $H$ is selfadjoint in $\mathcal{F}_-$.

Consider the same orthogonal set $\{f_k\}_{k\in\mathbb{N}}$ as a set of vectors in $\mathcal{L}_+ \subseteq \mathcal{L}$ and define

$$f_{-k} := \tau f_k \quad , \qquad \forall\ k \in \mathbb{N}\ .$$

Then, the set $\{f_k\}_{k\in L}$ with $L := \mathbb{N} \cup (-\mathbb{N})$ is an orthonormal basis in $\mathcal{L}$ and is called a <u>self-dual basis</u> of $\mathcal{L}$. With respect to this basis, it is possible to reexpress $H$ in the form

$$H := \sum_{k,k'\in L} \langle f_k \,|\, M f_{k'}\rangle_{\mathcal{L}}\, B(f_k)B^*(f_{k'})\ , \tag{3.202}$$

where $M$ is the block-matrix given by

$$M = \begin{pmatrix} c & b \\ b^* & \mathbf{0} \end{pmatrix} \tag{3.203}$$

and $b$ is the quadratic operator in $\mathcal{H}^1$, given by

$$\langle f_k \,|\, b f_{k'}\rangle = b_{k,k'} \quad , \qquad \forall\ k, k' \in \mathbb{N}\ . \tag{3.204}$$

(The numbers $b_{k,k'}$ are assumed to be zero if $k \notin I$ or $k' \notin I$.)

It is now easy to express the action of a homogeneous Bogoliubov transformation $w$, possessing a unitary implementation $U_w$, on $H$, as follows:

$$U_w H U_w^* = \sum_{k,k' \in L} \left\langle \tilde{f}_k \,\middle|\, w M w^* \tilde{f}_{k'} \right\rangle B(\tilde{f}_k) B^*(\tilde{f}_{k'}) \ , \quad \text{with} \qquad \tilde{f}_k := w f_k \ . \tag{3.205}$$

Note that $\{\tilde{f}_k\}_{k \in L}$ is again a self-dual basis in $\mathcal{L}$.

We now show how the generators $B(\cdot)$ of the self-dual algebra transform under the action of the strongly continuous unitary groups associated to such quadratic operators.

**Theorem 3.33.** *Let $H$ be a selfadjoint operator in $\mathcal{F}_-$ of the form* (3.202) *and assume that there exists a homogeneous Bogoliubov transformation $w$, possessing a unitary implementation $U_w$, such that*

$$\tilde{H} := U_w H U_w^* = \mathrm{d}\mathbf{G}(c) \ , \tag{3.206}$$

*for some one-particle operator $c = c^*$ in $\mathcal{H}^1$, not necessarily bounded. Then $M - \tau M \tau$ is selfadjoint in $\mathcal{L}$ and we have*

$$e^{itH} B(f) e^{-itH} = B\big(e^{it(M - \tau M \tau)} f\big) \ , \tag{3.207}$$

*for all $f \in \mathcal{L}$.*

*Proof:* By hypothesis we have

$$M - \tau M \tau = w^* C w \ , \quad \text{with} \qquad C = \begin{pmatrix} c & \mathbf{0} \\ \mathbf{0} & -\bar{c} \end{pmatrix} \ . \tag{3.208}$$

It is thus clear that $M - \tau M \tau$ is selfadjoint, since $C$ is selfadjoint, since $c$ is. We now proceed to prove the claimed relation in the special case $\tilde{H} = H$, or, equivalently $w = \mathbf{1}$.

$c$ is selfadjoint in $\mathcal{H}^1$. Therefore it possesses a dense family $\mathcal{D}_c \subseteq \mathcal{H}^1$ of analytic vectors and hence $C$ possesses a dense family $\mathcal{D}_C \subseteq \mathcal{L}$ of analytic vectors. As we have seen in the proof of Theorem 1.2, there is also a dense family of analytic vectors of $H$, given by

$$\mathcal{D}_H := \mathrm{span}\Big\{ \psi \in F_- \;\Big|\; \psi^{(n)} = \mathcal{S}_- \varphi_1 \otimes \cdots \otimes \varphi_n \text{ for all } n \in \mathbb{N}_0 \text{ and } \varphi_1, \ldots, \varphi_n \in \mathcal{D}_c \Big\} \ . \tag{3.209}$$

For any $\psi \in \mathcal{D}_H$ and any $f \in \mathcal{D}_C$, we also have $B(f)\psi \in \mathcal{D}_H$ and hence, by Lemma D.3, we have

$$H^k B(f) \psi = \sum_{l=0}^{k} \binom{k}{l} B(C^l f) H^{k-l} \psi \quad , \qquad \forall\, \psi \in \mathcal{D}_H \ . \tag{3.210}$$

With the help of Lemmas D.1 and D.3, we can now conclude

$$\begin{aligned} e^{itH} B(f) \psi &= \lim_{K \to \infty} \sum_{k=0}^{K} \frac{1}{k!} (it)^k H^k B(f) \psi \\ &= \lim_{K \to \infty} \sum_{k=0}^{K} \frac{1}{k!} (it)^k \sum_{l=0}^{k} \binom{k}{l} B(C^l f) H^{k-l} \psi \\ &= \lim_{K \to \infty} \sum_{k=0}^{K} \sum_{l=0}^{k} \frac{(it)^l}{l!} B(C^l f) \frac{(it)^{k-l}}{(k-l)!} H^{k-l} \psi \ . \end{aligned} \tag{3.211}$$

We now show that the sums on the right hand side may be decoupled in a manner similar to the Cauchy Product Formula. Namely, we have, as in the boson case (see p. 52),

$$\begin{aligned}
\text{l. h. s.} := \Bigg\| \sum_{k=0}^{K} \sum_{l=0}^{k} \frac{(it)^l}{l!} B(C^l f) \frac{(it)^{k-l}}{(k-l)!} H^{k-l} \psi^{(n)} \\
- \sum_{l=0}^{K} \frac{(it)^l}{l!} B(C^l f) \sum_{k=0}^{K} \frac{(it)^k}{k!} H^k \psi^{(n)} \Bigg\| \\
\leq \sum_{\frac{K}{2} < l \leq K} \left\| \frac{(it)^l}{l!} B(C^l f) \right\| \cdot \sum_{k=0}^{K} \left\| \frac{(it)^k}{k!} H^k \psi^{(n)} \right\| \\
+ \sum_{l=0}^{K} \left\| \frac{(it)^l}{l!} B(C^l f) \right\| \cdot \sum_{\frac{K}{2} < k \leq K} \left\| \frac{(it)^k}{k!} H^k \psi^{(n)} \right\| , \qquad (3.212)
\end{aligned}$$

for all $\psi \in \mathcal{D}_H$. Since

$$\left\| B(C^l f) \right\| \leq 2 \left\| C^l f \right\| \quad , \qquad \forall\ f \in \mathcal{D}_C \ , \qquad (3.213)$$

we can estimate further

$$\begin{aligned}
\text{l. h. s.} \leq 2 \sum_{\frac{K}{2} < l \leq K} \frac{t^l}{l!} \left\| C^l f \right\| \cdot \sum_{k=0}^{K} \frac{t^k}{k!} \left\| H^k \psi^{(n)} \right\| \\
+ 2 \sum_{l=0}^{K} \frac{t^l}{l!} \left\| C^l f \right\| \cdot \sum_{\frac{K}{2} < k \leq K} \frac{t^k}{k!} \left\| H^k \psi^{(n)} \right\| \ . \qquad (3.214)
\end{aligned}$$

Obviously, the right hand side of this estimate converges to zero as $K \to \infty$ due to the analyticity properties of $f$ and $\psi$. Hence, we have

$$e^{itH} B(f) \psi = B(e^{itC} f) e^{itH} \psi \quad , \qquad \forall\ \psi \in \mathcal{D}_H,\ f \in \mathcal{D}_C \ . \qquad (3.215)$$

By the fact that $\mathcal{D}_H$ is dense in $\mathcal{F}_-$ and $\mathcal{D}_C$ is dense in $\mathcal{L}$ and moreover by the continuity of the mapping $f \mapsto B(f)$, we may conclude

$$e^{itH} B(f) e^{-itH} = B(e^{itC}) \ . \qquad (3.216)$$

We have thus proved the theorem in the case $\tilde{H} = H$. As for the general case, we remark

$$\begin{aligned}
e^{itH} B(f) e^{-itH} = U_w^* e^{it\tilde{H}} U_w B(f) U_w^* e^{-it\tilde{H}} U_w = U_w^* e^{it\tilde{H}} B(wf) e^{-it\tilde{H}} U_w \\
= U_w^* B(e^{itC} wf) U_w = B(w^* e^{itC} wf) = B(e^{itw^* C w} f) \ . \qquad (3.217)
\end{aligned}$$

We are done since $M - \tau M \tau = w^* C w$. □

### 3.2.4 The Generating Functional

This subsection is dedicated to the calculation of the fermionic generating functional. We would like to view this 'functional' as a certain element of the Grassmann Algebra, depending on an integer $\kappa$ and a suitably chosen quadratic operator $H$. We introduce the Grassmann Algebra and briefly discuss its basic features in Appendix C.

Let us fix for this subsection an orthonormal basis $\{f_k\}_{k\in\mathbb{N}}$ in $\mathcal{H}^1$, and agree to denote for the generators $\xi(\cdot)$ and $\xi^*(\cdot)$ of any Grassmann Algebra over $\mathcal{H}^1$:

$$(\xi^*)_\kappa \cdot (\xi)_\kappa := \sum_{k=1}^{\kappa} \xi^*(f_k)\xi(f_k) \qquad \text{and} \qquad (\xi)_\kappa \cdot (\xi^*)_\kappa := \sum_{k=1}^{\kappa} \xi(f_k)\xi^*(f_k) \tag{3.218}$$

and also

$$(\xi^*)^{\underline{s}}_\kappa := \big(\xi^*(f_1)\big)^{s_1} \cdots \big(\xi^*(f_\kappa)\big)^{s_\kappa} \qquad \text{and} \qquad (\xi)^{\underline{s}}_\kappa := \big(\xi(f_\kappa)\big)^{s_\kappa} \cdots \big(\xi(f_1)\big)^{s_1} \ , \tag{3.219}$$

for all $\kappa \in \mathbb{N}$ and all multi-indices $\underline{s} \in \{0,1\}^\kappa$. These notations are explained in more detail in Section C.1. Now let $\eta(\cdot)$ and $\eta^*(\cdot)$ generate such a Grassmann Algebra over $\mathcal{H}^1$. We then define, for any $\kappa \in \mathbb{N}$ and any suitable quadratic operator $H$, the generating functional by

$$\mathcal{G}_{H,\kappa} := e^{\frac{1}{2}(\eta^*)_\kappa\cdot(\eta)_\kappa} \sum_{\underline{m},\underline{n}\in\{0,1\}^\kappa} (\eta)^{\underline{m}}_\kappa (\eta^*)^{\underline{n}}_\kappa \frac{\mathrm{tr}\left((a)^{\underline{n}}_\kappa (a^*)^{\underline{m}}_\kappa P_\kappa e^{-H} P_\kappa\right)}{\mathrm{tr}(P_\kappa e^{-H})} \ , \tag{3.220}$$

where we have introduced the orthogonal projection $P_\kappa$ in $\mathcal{F}_-$

$$P_\kappa := \mathbf{G}\left(P_{\mathrm{span}\{f_1,\ldots,f_\kappa\}}\right) \ , \tag{3.221}$$

where $P_{\mathrm{span}\{f_1,\ldots,f_\kappa\}}$ is the orthogonal projection in $\mathcal{H}^1$ given by

$$P_{\mathrm{span}\{f_1,\ldots,f_\kappa\}} f_l := \begin{cases} f_l & \text{if } l \leq \kappa \\ 0 & \text{else} \end{cases} \ , \qquad \forall\, l \in \mathbb{N} \ . \tag{3.222}$$

Also, we have denoted

$$(a^*)^{\underline{n}}_\kappa := \big(a^*(f_1)\big)^{n_1} \cdots \big(a^*(f_\kappa)\big)^{n_\kappa} \qquad \text{and} \qquad (a)^{\underline{n}}_\kappa := \big(a(f_\kappa)\big)^{n_\kappa} \cdots \big(a(f_1)\big)^{n_1} \ , \tag{3.223}$$

for all multi-indices $\underline{n} \in \{0,1\}^\kappa$. We later specify for which quadratic operators $H$ the right hand side of (3.220) actually makes sense. In order to motivate Definition (3.220) of the generating functional and to establish contact with the bosonic theory, we point out that this expression may formally be written as

$$\mathcal{G}_{H,\kappa} = \frac{\mathrm{tr}\left(e^{\sum_{k=1}^{\kappa} \eta^*(f_k)a(f_k)+\eta(f_k)a^*(f_k)} P_\kappa e^{-H} P_\kappa\right)}{\mathrm{tr}\left(e^{-H} P_\kappa\right)} \ . \tag{3.224}$$

Equality of (3.220) and (3.224) is established by first decoupling in (3.224) the sum in the exponential with the aid of the Baker-Cambell-Hausdorff Relation, see, e. g., [32],

$$e^{\sum_{k=1}^{\kappa} \eta(f_k)a^*(f_k)+\eta^*(f_k)a(f_k)} = e^{\frac{1}{2}(\eta^*)_\kappa\cdot(\eta)_\kappa} e^{\sum_{k=1}^{\kappa} \eta(f_k)^* a(f_k)} e^{\sum_{k=1}^{\kappa} \eta(f_k)a^*(f_k)} \tag{3.225}$$

and expanding the resulting exponentials by formulas analogous to (C.21). Here, we have supposed that all Grassmann variables are to be pulled out of the trace to the left. However, it should be said that formula (3.224), as it stands, does not make sense, since nothing has been said about how to take a Fock space trace of an element of the Grassmann extended CAR Algebra. We view relation (3.224) as mere mnemotechniques. (See however Section C.3.)

We proceed to introduce the tools we need to calculate the value of $\mathcal{G}_{H,\kappa}$.

Similarly to identity (3.139), we use a fundamental fact about Gaussian integrals of Grassmann variables as a tool to calculate the value of the generating functional.

**Lemma 3.34.** *Let $\xi(\cdot)$ generate a Grassmann Algebra over $\mathcal{H}^1$. Using the notation introduced in Section C.1, we have*

$$\delta_{\underline{m},\underline{n}} = \int e^{(\xi^*)_\kappa \cdot (\xi)_\kappa} (\xi^*)^{\underline{m}}_\kappa (\xi)^{\underline{n}}_\kappa \, (d\xi)_\kappa (d\xi^*)_\kappa \; = \; \int e^{(\xi)_\kappa \cdot (\xi^*)_\kappa} (\xi)^{\underline{m}}_\kappa (\xi^*)^{\underline{n}}_\kappa \, (d\xi^*)_\kappa (d\xi)_\kappa \ , \tag{3.226}$$

*for any multi-indices $\underline{m}, \underline{n} \in \{0,1\}^\kappa$.*

The Grassmann integral appearing in (3.226) is introduced in (C.7).

*Proof:* Use identities (C.21), write out the integrals in terms of iterated integrals and finally use (C.24). □

On the basis of this lemma, the next two lemmas are easily proved. In order to formulate these, we define, for any finite occupation $\underline{n}$ with

$$\underline{n} \in \{0,1\}^{\mathbb{N}} \qquad \text{and} \qquad |\,\underline{n}\,| := \sum_{j \in \mathbb{N}} n_j < \infty \ , \tag{3.227}$$

the normalized vector $\psi_{\underline{n}}$ in the Fock space $\mathcal{F}_-$:

$$\psi_{\underline{n}} := \sqrt{|\,\underline{n}\,|!}\, \mathcal{S}_- \big( (f_1)^{\otimes n_1} \otimes (f_2)^{\otimes n_2} \otimes \cdots \big) \qquad , \qquad \psi_{\underline{0}} := \Omega \tag{3.228}$$

or, equivalently,

$$\psi_{\underline{n}} := \big(a^*(f_1)\big)^{n_1} \big(a^*(f_2)\big)^{n_2} \cdots \Omega \ . \tag{3.229}$$

Obviously, any finite occupation number $\underline{n}$ may be viewed as a multi-index in $\{0,1\}^\kappa$, for all $\kappa$ such that $n_j = 0$, for all $j > \kappa$. Conversely any multi-index $\underline{s}$ in $\{0,1\}^\kappa$ may be viewed as a finite occupation number by setting $s_j = 0$, for all $j > \kappa$.

**Lemma 3.35.** *Let $\xi(\cdot)$ and $\xi^*(\cdot)$ generate a Grassmann Algebra over $\mathcal{H}^1$. Then, for any trace-class operator $A$ in $\mathcal{F}_-$, the following trace formula holds:*

$$\mathrm{tr}(A) = \lim_{\kappa \to \infty} \int \exp\big((\xi^*)_\kappa \cdot (\xi)_\kappa\big) \widehat{A}_\kappa(\xi^*, \xi) (d\xi)_\kappa (d\xi^*)_\kappa \ , \tag{3.230}$$

*where we have introduced*

$$\widehat{A}_\kappa(\xi^*, \xi) \ := \sum_{\underline{n}, \underline{m} \in \{0,1\}^\kappa} (\xi^*)^{\underline{n}}_\kappa \big\langle \psi_{\underline{n}} \,\big|\, A \psi_{\underline{m}} \big\rangle \, (\xi)^{\underline{m}}_\kappa \ . \tag{3.231}$$

For any operator $A$ in the Fock space $\mathcal{F}_-$ such that

$$V_\kappa := P_\kappa \mathcal{F}_- \ \subseteq \ \mathcal{D}(A) \quad , \qquad \forall\, \kappa \in \mathbb{N} \tag{3.232a}$$

and moreover

$$AV_\kappa \subseteq V_\kappa \ , \tag{3.232b}$$

we shall call the collection of Grassmann quantities $\{\widehat{A}_\kappa(\xi^*, \xi)\}_{\kappa\in\mathbb{N}}$ defined in (3.231) the symbols of the operator $A$. $P_\kappa$ is defined in (3.221). We do not need to make any assumptions whatsoever on the convergence of the sequence of symbols. They contain all the information on the operator $A$ we shall utilize.

**Lemma 3.36.** *Let $\xi(\cdot)$ and $\xi^*(\cdot)$ generate a Grassmann Algebra over $\mathcal{H}^1$. Then, for any two vectors $\psi, \phi \in \mathcal{F}_-$, we have the following decomposition of the identity:*

$$\begin{aligned}\langle \psi \,|\, \phi \rangle = \lim_{\kappa\to\infty} \int \exp\big((\xi)_\kappa \cdot (\xi^*)_\kappa\big) &\left\{ \sum_{\underline{m}\in\{0,1\}^\kappa} \langle \psi \,|\, \psi_{\underline{m}} \rangle \, (\xi)^{\underline{m}}_\kappa \right\} \\ \cdot &\left\{ \sum_{\underline{n}\in\{0,1\}^\kappa} (\xi^*)^{\underline{n}}_\kappa \, \langle \psi_{\underline{n}} \,|\, \phi \rangle \right\} (d\xi)^*_\kappa (d\xi)_\kappa \ .\end{aligned} \tag{3.233}$$

The expressions in the curly braces in (3.233) may be expressed in terms of the following linear functionals $\chi_\kappa$ on fermionic fock space $\mathcal{F}_-$ with values in the Grassmann Algebra generated by $\xi(\cdot)$, by

$$\phi \mapsto \chi_\kappa(\phi) \ := \sum_{\underline{n}\in\{0,1\}^\kappa} (\xi^*)^{\underline{n}}_\kappa \, \langle \psi_{\underline{n}} \,|\, \phi \rangle \tag{3.234}$$

and its adjoint $\chi^*_\kappa$. The adjoint functionals $\chi^*_\kappa$ may be viewed as anti-linear functionals, defined by taking the algebraic adjoints of the values of $\chi_\kappa$. Note that formally we may write $\chi_\kappa$ and $\chi^*_\kappa$, respectively, in the following form:

$$\chi_\kappa(\phi) = \big\langle \exp\big(-(\xi)_\kappa \cdot (a^*)_\kappa\big)\Omega \,|\, \phi \big\rangle \quad , \qquad \chi^*_\kappa(\psi) = \big\langle \psi \,\big|\, \exp\big(-(\xi)_\kappa \cdot (a^*)_\kappa\big)\Omega \big\rangle \ . \tag{3.235}$$

It is now clear, why the functionals $\chi_\kappa$ and $\chi^*_\kappa$ are also called fermionic coherent states (see e. g. Ohnuki and Kashiwa [25], reprinted in [21]). For example, it is possible to express the symbols of an operator, see (3.231), as matrix elements in coherent states. However, we would like to view expression (3.235) as mere mnemotechniques and caution the reader of using these notions too freely. In particular we point out that some linearity properties of the scalar product with respect to Grassmann variables have to be stipulated, in order to make sense of these relations.

The following lemma shows that in some generalized sense, the coherent states are 'eigen-functionals' of the particle annihilation operator $a(\cdot)$.

**Lemma 3.37.** *For any linear combination $g \in \mathcal{H}^1$ of the $\kappa$ first elements $f_1, \ldots, f_\kappa$ of the orthonormal basis chosen and any vector $\phi \in \mathcal{F}_-$, the following relation holds true*

$$\chi_\kappa\big(a^*(g)\phi\big) = \xi^*(g) \cdot \chi_\kappa(\phi) \ , \tag{3.236}$$

*or, more generally, for any $g \in \mathcal{H}^1$, we have*

$$\chi_\kappa\big(a^*(g)\phi\big) = \xi^*\left(P_{\mathrm{span}\{f_1,\ldots,f_\kappa\}}g\right) \cdot \chi_\kappa(\phi) \ . \tag{3.237}$$

*Proof:* By the definition of the coherent state $\chi_\kappa$ we have, for any $g \in \mathcal{H}^1$ and any $\phi \in \mathcal{F}_-$,

$$\begin{aligned}
\chi_\kappa\big(a^*(g)\phi\big) &= \sum_{\underline{n}\in\{0,1\}^\kappa} (\xi^*)^{\underline{n}}_{\kappa} \,\big\langle a(g)\psi_{\underline{n}} \,|\, \phi \big\rangle \\
&= \sum_{\underline{n}\in\{0,1\}^\kappa} \big(\xi^*(f_1)\big)^{n_1}\cdots\big(\xi^*(f_\kappa)\big)^{n_\kappa} \sum_{l=1}^{\kappa} \delta_{n_l,1}(-1)^{n_1+\cdots+n_{l-1}} \langle f_l \,|\, g\rangle \big\langle \psi_{\underline{n}-\underline{e}^l} \,|\, \phi\big\rangle \\
&= \sum_{l=1}^{\kappa} \langle f_l \,|\, g\rangle \cdot \xi^*(f_l) \sum_{\underline{n}\in\{0,1\}^\kappa} \delta_{n_l,1}(\xi^*)^{\underline{n}-\underline{e}^l}_{\kappa} \big\langle \psi_{\underline{n}-\underline{e}^l} \,|\, \phi\big\rangle \\
&= \xi^*\left(\sum_{l=1}^{\kappa} \langle f_l \,|\, g\rangle\, f_l\right) \chi_\kappa(\phi) \ ,
\end{aligned}$$

where we have used the notation $\underline{e}^l := \{\delta_{l,j}\}_{j\in\mathbb{N}}$. Note that in the last step we have made use of $\xi^*(f_l)^2 = 0$. □

We proceed to show how the symbols of operators in $\mathcal{F}_-$ can be calculated. To this end, we define the <u>projections $\{A_\kappa\}_{\kappa\in\mathbb{N}}$ of an operator $A$ in $\mathcal{F}_-$</u> obeying (3.232) in the following manner:

$$A_\kappa := P_\kappa A P_\kappa \quad , \qquad \forall\ \kappa \in \mathbb{N} \ , \tag{3.238}$$

with $P_\kappa$ as in (3.221). Note that if $A \in \mathcal{B}(\mathcal{F}_-)$, then $A$ is uniquely determined by its sequence of projections, since

$$A\psi = \lim_{\kappa\to\infty} A_\kappa \psi \quad , \qquad \forall\ \psi \in \mathcal{F}_- \ . \tag{3.239}$$

Obviously, any sequence of projections $\{A_\kappa\}_{\kappa\in\mathbb{N}}$ of a given operator $A$ satisfies certain consistency conditions (this is however unimportant for us).

Now, each $A_\kappa$ lies in the $C^*$-algebra generated by $a(f_1), \ldots, a(f_\kappa)$ and their adjoints. Since this algebra is a finite dimensional vector space, any $A_\kappa$ can be represented as a normal-ordered polynomial

$$p_\kappa\big(a^*(f_1), \ldots, a^*(f_\kappa); a(f_\kappa), \ldots, a(f_1)\big) \ , \tag{3.240}$$

i. e., as a polynomial with the property that in each of its monomials all particle creation operators $a^*(\cdot)$ stand to the left of all particle annihilation operators $a(\cdot)$. For notational convenience, we also denote (3.240) simply by

$$p_\kappa(a^*; a) \ . \tag{3.241}$$

**Lemma 3.38.** *Let $A$ be an operator in $\mathcal{F}_-$ obeying* (3.232)*, and denote by $A_\kappa$ and $p_\kappa$ the projections of $A$ and their normal-ordered forms as in relations* (3.238) *and* (3.240)*, respectively. The symbols of $A$ with respect to a set of Grassmann variables, corresponding to the Grassmann generator $\xi(\cdot)$, are then given by:*

$$\widehat{A}_\kappa(\xi^*; \xi) = p_\kappa\,(\xi^*; \xi) \exp\big((\xi^*)_\kappa \cdot (\xi)_\kappa\big) \quad , \qquad \forall\ \kappa \in \mathbb{N} \ . \tag{3.242}$$

*Proof:* By linearity, we may assume that all the normal-ordered forms $p_\kappa$ of the projections $A_\kappa$ of $A$ are monomials. We express the fact that they are assumed to be normal-ordered, by noting that each $p_\kappa$ can be written in the form

$$p_\kappa(a^*; a) = r_\kappa(a^*) s_\kappa(a) \ , \tag{3.243}$$

for suitable monomials $r_\kappa$ and $s_\kappa$ in the operators $a^*(f_1), \ldots, a^*(f_\kappa)$ and $a(f_1), \ldots, a(f_\kappa)$, respectively. By the definition of the symbols of the operator $A$ we have

$$\begin{aligned}\widehat{A}_\kappa(\xi^*, \xi) &= \sum_{\underline{m},\underline{n} \in \{0,1\}^\kappa} (\xi^*)_\kappa^{\underline{n}} \left\langle \psi_{\underline{n}} \,\middle|\, A\psi_{\underline{m}} \right\rangle (\xi)_\kappa^{\underline{m}} \\ &= \sum_{\underline{m},\underline{n} \in \{0,1\}^\kappa} (\xi^*)_\kappa^{\underline{n}} \left\langle \psi_{\underline{n}} \,\middle|\, r_\kappa(a^*) s_\kappa(a) \psi_{\underline{m}} \right\rangle (\xi)_\kappa^{\underline{m}} . \end{aligned} \tag{3.244}$$

From this we obtain, on using Lemma 3.37, that

$$\begin{aligned}\widehat{A}_\kappa(\xi^*, \xi) &= r_\kappa(\xi^*) \left( \sum_{\underline{m},\underline{n} \in \{0,1\}^\kappa} (\xi^*)_\kappa^{\underline{n}} \left\langle \psi_{\underline{n}} \,\middle|\, \psi_{\underline{m}} \right\rangle (\xi)_\kappa^{\underline{m}} \right) s_\kappa(\xi) \\ &= r_\kappa(\xi^*) s_\kappa(\xi) \sum_{\underline{n} \in \{0,1\}^\kappa} (\xi^*)_\kappa^{\underline{n}} (\xi)_\kappa^{\underline{n}} \; = \; p_\kappa(\xi^*; \xi) \exp\big( (\xi^*)_\kappa \cdot (\xi)_\kappa \big) . \end{aligned} \tag{3.245}$$

In the last step we have used (C.21). □

As a last preparation, we show how to calculate the symbols of a product of operators.

**Lemma 3.39.** *Let $A^{(1)}, \ldots, A^{(N)}$ be operators, all of them obeying* (3.232)*. The $A := A^{(1)} \cdots A^{(N)}$ obeys* (3.232) *and*

$$\begin{aligned}\widehat{A}_\kappa(\xi^*, \xi) = \int \exp\left( \sum_{l=1}^{N-1} (\xi_l)_\kappa \cdot (\xi_l^*)_\kappa \right) \widehat{A}_\kappa^{(1)}(\xi^*, \xi_1) \widehat{A}_\kappa^{(2)}(\xi_1^*, \xi_2) \cdots \\ \cdots \widehat{A}_\kappa^{(N)}(\xi_{N-1}^*, \xi) \, (d\xi_1^*)_\kappa (d\xi_1)_\kappa \cdots (d\xi_{N-1}^*)_\kappa (d\xi_{N-1})_\kappa \, , \end{aligned} \tag{3.246}$$

*where we have introduced $N$ sets of Grassmann variables, corresponding to the generators $\xi(\cdot), \xi_1(\cdot), \ldots, \xi_{N-1}(\cdot)$.*

*Proof:* Obviously $A$ obeys (3.232). By the definition of the symbols of the operator $A$, we obtain for the left hand side (l. h. s.) of the claim

$$\text{l. h. s.} = \sum_{\underline{m},\underline{n} \in \{0,1\}^\kappa} (\xi^*)_\kappa^{\underline{m}} \left\langle \psi_{\underline{m}} \,\middle|\, A^{(1)} \cdots A^{(N)} \psi_{\underline{n}} \right\rangle (\xi)_\kappa^{\underline{n}} \tag{3.247}$$

and by Lemma 3.36

$$\begin{aligned}\left\langle \psi_{\underline{m}} \,\middle|\, A^{(1)} \cdots A^{(N)} \psi_{\underline{n}} \right\rangle = \lim_{\kappa_1 \to \infty} \sum_{\underline{m}_1,\underline{n}_1 \in \{0,1\}^{\kappa_1}} \int \exp\big( (\xi_1)_{\kappa_1} \cdot (\xi_1^*)_{\kappa_1} \big) \\ \cdot \left\langle \psi_{\underline{m}} \,\middle|\, A^{(1)} \psi_{\underline{n}_1} \right\rangle (\xi_1)_{\kappa_1}^{\underline{n}_1} (\xi_1^*)_{\kappa_1}^{\underline{m}_1} \left\langle \psi_{\underline{m}_1} \,\middle|\, A^{(2)} \cdots A^{(N)} \psi_{\underline{n}} \right\rangle (d\xi_1^*)_{\kappa_1} (d\xi_1)_{\kappa_1} . \end{aligned} \tag{3.248}$$

Since, by hypothesis, $A^{(1)}\psi_{\underline{m}}$ and $A^{(2)} \cdots A^{(N)}\psi_{\underline{n}}$ are in the range of $P_\kappa$, the limit as $\kappa_1 \to \infty$ is attained at $\kappa_1 = \kappa$. Inserting (3.248) into (3.247), we obtain

$$\text{l. h. s.} = \int \exp\big( (\xi_1)_\kappa \cdot (\xi_1^*)_\kappa \big) \, \widehat{A}_\kappa^{(1)}(\xi^*, \xi_1) \big( \widehat{A^{(2)} \cdots A^{(N)}} \big)_\kappa (\xi_1^*, \xi) \, (d\xi_1^*)_\kappa (d\xi_1)_\kappa . \tag{3.249}$$

The claim of the lemma follows by applying the above argument $N-1$ times. □

We are now ready to calculate the value of the generating functional. Again we start with a selfadjoint Hamiltionian $H$ in $\mathcal{F}_-$, which is the second quantization of a one-particle operator. We generalize this later.

**Lemma 3.40.** *Let $H$ be a selfadjoint, nonnegative operator in $\mathcal{F}_-$ obeying* (3.232)*. On introducing two sets of Grassmann variables, corresponding to the Grassmann generators $\eta(\cdot)$ and $\xi(\cdot)$, respectively, we obtain the following relation*

$$\sum_{\underline{m},\underline{n}\in\{0,1\}^\kappa} (\eta)^{\underline{m}}_\kappa(\eta^*)^{\underline{n}}_\kappa \operatorname{tr}\left((a)^{\underline{n}}_\kappa(a^*)^{\underline{m}}_\kappa P_\kappa e^{-H}P_\kappa\right)$$
$$= \int \exp\Big((\xi^*)_\kappa\cdot(\xi)_\kappa - (\eta^*)_\kappa\cdot(\xi)_\kappa - (\xi^*)_\kappa\cdot(\eta)_\kappa\Big)\widehat{(e^{-H})}_\kappa(\xi^*;\xi)\,(d\xi)_\kappa(d\xi^*)_\kappa \quad (3.250)$$

*Proof:* It is clear that $e^{-H}$ also obeys (3.232). By the trace formula (3.230), we obtain for the left hand side (l. h. s.) of the claim, after introducing a third set of Grassmann variables corresponding to the Grassmann generator $\zeta(\cdot)$,

$$\text{l. h. s.} = \sum_{\underline{m},\underline{n}\in\{0,1\}^\kappa} (\eta)^{\underline{m}}_\kappa(\eta^*)^{\underline{n}}_\kappa \int \exp\left((\zeta^*)_\kappa\cdot(\zeta)_\kappa\right)$$
$$\sum_{\underline{r},\underline{s}\in\{0,1\}^\kappa} (\zeta^*)^{\underline{r}}_\kappa \left\langle (a^*)^{\underline{n}}_\kappa\psi_{\underline{r}} \,\middle|\, (a^*)^{\underline{m}}_\kappa e^{-H}\psi_{\underline{s}}\right\rangle (\zeta)^{\underline{s}}_\kappa\,(d\zeta)_\kappa(d\zeta^*)_\kappa \quad (3.251)$$

and with the help of the decomposition of the identity, given by relation (3.233), we have

$$\left\langle (a^*)^{\underline{n}}_\kappa\psi_{\underline{r}} \,\middle|\, (a^*)^{\underline{m}}_\kappa e^{-H}\psi_{\underline{s}}\right\rangle = \lim_{\kappa'\to\infty}\int \exp\left((\xi)_{\kappa'}\cdot(\xi^*)_{\kappa'}\right)$$
$$\left\{\sum_{\underline{p}\in\{0,1\}^{\kappa'}} \left\langle (a^*)^{\underline{n}}_\kappa\psi_{\underline{r}} \,\middle|\, \psi_{\underline{p}}\right\rangle (\xi)^{\underline{p}}_{\kappa'}\right\}\left\{\sum_{\underline{q}\in\{0,1\}^{\kappa'}} (\xi^*)^{\underline{q}}_{\kappa'}\left\langle \psi_{\underline{q}} \,\middle|\, (a^*)^{m}_\kappa e^{-H}\psi_{\underline{s}}\right\rangle\right\}(d\xi^*)_{\kappa'}(d\xi)_{\kappa'}\ . \quad (3.252)$$

As the next ingredient to our proof, we use Lemma 3.37 to see that

$$\left\langle (a^*)^{\underline{n}}_\kappa\psi_{\underline{r}} \,\middle|\, (a^*)^{\underline{m}}_\kappa e^{-H}\psi_{\underline{s}}\right\rangle = \lim_{\kappa'\to\infty}\int \exp\left((\xi)_{\kappa'}\cdot(\xi^*)_{\kappa'}\right)$$
$$(\xi)^{\underline{r}}_\kappa(\xi)^{\underline{n}}_\kappa(\xi^*)^{\underline{m}}_\kappa\left\{\sum_{\underline{q}\in\{0,1\}^{\kappa'}} (\xi^*)^{\underline{q}}_{\kappa'}\left\langle \psi_{\underline{q}} \,\middle|\, e^{-H}\psi_{\underline{s}}\right\rangle\right\}(d\xi^*)_{\kappa'}(d\xi)_{\kappa'}\ , \quad (3.253)$$

for all multi-indices $\underline{m},\underline{n},\underline{r},\underline{s}\in\{0,1\}^\kappa$. Very importantly, we observe that in the sum over $\underline{q}\in\{0,1\}^{\kappa'}$, only those terms corresponding to such a $\underline{q}$ with the property

$$q_j = 0 \quad , \qquad \forall\, j>\kappa \quad (3.254)$$

contribute to the integral, since all the remaining $\kappa'-\kappa$ integrations yield a factor 1. Hence,

$$\text{l. h. s.} = \sum_{\underline{m},\underline{n}\in\{0,1\}^\kappa} (\eta)^{\underline{m}}_\kappa(\eta^*)^{\underline{n}}_\kappa \int \exp\left((\zeta^*)_\kappa\cdot(\zeta)_\kappa + (\xi)_\kappa\cdot(\xi^*)_\kappa\right)$$
$$\sum_{\underline{r},\underline{s},\underline{q}\in\{0,1\}^\kappa} (\zeta^*)^{\underline{r}}_\kappa(\xi)^{\underline{r}}_\kappa(\xi)^{\underline{n}}_\kappa(\xi^*)^{\underline{m}}_\kappa(\xi^*)^{\underline{q}}_\kappa\left\langle \psi_{\underline{q}} \,\middle|\, e^{-H}\psi_{\underline{s}}\right\rangle (\zeta)^{\underline{s}}_\kappa\,(d\xi^*)_\kappa(d\xi)_\kappa(d\zeta)_\kappa(d\zeta^*)_\kappa\ . \quad (3.255)$$

Repeatedly using relations (C.21) and rule (C.9), we obtain

$$\begin{aligned}
\text{l. h. s.} &= \int \exp\big((\zeta^*)_\kappa \cdot (\zeta)_\kappa + (\xi)_\kappa \cdot (\xi^*)_\kappa + (\zeta^*)_\kappa \cdot (\xi)_\kappa + (\eta^*)_\kappa \cdot (\xi)_\kappa + (\eta)_\kappa \cdot (\xi^*)_\kappa\big) \\
&\qquad \widehat{(e^{-H})}_\kappa(\xi^*;\zeta)\,(d\xi)_\kappa(d\zeta^*)_\kappa(d\zeta)_\kappa(d\xi^*)_\kappa \\
&= \int \exp\big((\zeta^*)_\kappa \cdot (\zeta)_\kappa + (\eta)_\kappa \cdot (\xi^*)_\kappa\big)\widehat{(e^{-H})}_\kappa(\xi^*;\zeta) \\
&\qquad \exp\big((\zeta^* - (\xi^* - \eta^*))_\kappa \cdot (\xi)_\kappa\big)\,(d\xi)_\kappa(d\zeta^*)_\kappa(d\zeta)_\kappa(d\xi^*)_\kappa\ .
\end{aligned}$$

From this, we arrive at the right hand side of the assertion by carrying out the integrations over the $\xi$ and $\zeta^*$ variables with the help of Lemma C.3 and by renaming the Grassmann variables according to $\zeta \mapsto \xi$. □

We observe that

$$\big\langle \psi_{\underline{m}} \,\big|\, e^{-H}\psi_{\underline{n}} \big\rangle = \lim_{N\to\infty} \Big\langle \psi_{\underline{m}} \Big| \big(\mathbf{1} - \tfrac{1}{N}H\big)^N \psi_{\underline{n}} \Big\rangle\ , \tag{3.256}$$

for all finite occupation numbers $\underline{n}, \underline{m} \in \{0,1\}^{\mathbb{N}}$ and $H = H^*$ obeying (3.232). Thus, in view of the definition of the symbols of $e^{-H}$ and due to the fact that the Grassmann integral in (3.250) is continuous, since it is a linear mapping in a finite dimensional vector space, we may write by Lemma 3.40

$$\begin{aligned}
(\star) &:= \sum_{\underline{m},\underline{n}\in\{0,1\}^\kappa} (\eta)^{\underline{m}}_\kappa (\eta^*)^{\underline{n}}_\kappa \operatorname{tr}\big((a)^{\underline{n}}_\kappa (a^*)^{\underline{m}}_\kappa P_\kappa e^{-H} P_\kappa\big) \\
&= \lim_{N\to\infty} \int \exp\left[(\xi^*)_\kappa \cdot (\xi)_\kappa - (\eta^*)_\kappa \cdot (\xi)_\kappa - (\xi^*)_\kappa \cdot (\eta)_\kappa + \sum_{l=1}^{N-1} (\xi_l)_\kappa \cdot (\xi_l^*)_\kappa\right] \\
&\qquad \widehat{\big(\mathbf{1} - \tfrac{1}{N}H\big)}_\kappa(\xi^*, \xi_1)\widehat{\big(\mathbf{1} - \tfrac{1}{N}H\big)}_\kappa(\xi_1^*, \xi_2)\cdots\widehat{\big(\mathbf{1} - \tfrac{1}{N}H\big)}_\kappa(\xi_{N-1}^*, \xi) \\
&\qquad\qquad (d\xi_1^*)_\kappa(d\xi_1)_\kappa\cdots(d\xi_{N-1}^*)_\kappa(d\xi_{N-1})_\kappa(d\xi)_\kappa(d\xi^*)_\kappa\ .
\end{aligned} \tag{3.257}$$

We have used Lemma 3.39 to expand the symbol of the operator $(\mathbf{1} - \frac{1}{N}H)^N$. On using Lemma 3.38 and denoting by $H_\kappa(a^*, a)$ the normal-ordered form of the projections $H_\kappa$ of $H$, we obtain

$$\begin{aligned}
(\star) = \lim_{N\to\infty} \int \exp\Bigg[&(\xi^*)_\kappa \cdot (\xi)_\kappa - (\eta^*)_\kappa \cdot (\xi)_\kappa - (\xi^*)_\kappa \cdot (\eta)_\kappa - \sum_{l=1}^{N-1} (\xi_l^*)_\kappa \cdot (\xi_l)_\kappa \\
&+ \sum_{l=2}^{N-1} (\xi_{l-1}^*)_\kappa \cdot (\xi_l)_\kappa + (\xi^*)_\kappa \cdot (\xi_1)_\kappa + (\xi_{N-1}^*)_\kappa \cdot (\xi)_\kappa\Bigg] \\
&\big(\mathbf{1} - \tfrac{1}{N}H_\kappa(\xi^*;\xi_1)\big)\cdots\big(\mathbf{1} - \tfrac{1}{N}H_\kappa(\xi_{N-1}^*;\xi)\big) \\
&(d\xi_1^*)_\kappa(d\xi_1)_\kappa\cdots(d\xi_{N-1}^*)_\kappa(d\xi_{N-1})_\kappa(d\xi)_\kappa(d\xi^*)_\kappa\ .
\end{aligned} \tag{3.258}$$

By first renaming the Grassmann variables according to $\xi \mapsto \xi_N$ and $\xi^* \mapsto \xi_0^*$ and subsequently renaming $\xi_k^* \mapsto \xi_{k+1}^*$, we obtain from this

$$(\star) = \lim_{N\to\infty} \int \exp\left[ -(\eta^*)_\kappa \cdot (\xi_N)_\kappa - (\xi_1^*)_\kappa \cdot (\eta)_\kappa + \sum_{l,l'=1}^{N} Q_{l,l'} (\xi_l^*)_\kappa \cdot (\xi_{l'})_\kappa \right]$$
$$\left(\mathbf{1} - \tfrac{1}{N} H_\kappa(\xi_1^*, \xi_1)\right) \cdots \left(\mathbf{1} - \tfrac{1}{N} H_\kappa(\xi_N^*, \xi_N)\right) \prod_{j=1}^{N} \left((d\xi_j)_\kappa (d\xi_j^*)_\kappa\right) \ , \quad (3.259)$$

where we have denoted by $Q$ the following $N \times N$ matrix

$$Q := \begin{pmatrix} 1 & & & 1 \\ -1 & \ddots & & \\ & \ddots & \ddots & \\ & & -1 & 1 \end{pmatrix} . \quad (3.260)$$

In arriving at expression (3.259), we have changed the order of integration according to the following scheme: After renaming the Grassmann variables as indicated, we have concluded that

$$\prod_{j=1}^{N-1} \left((d\xi_{j+1}^*)_\kappa (d\xi_j)_\kappa\right) (d\xi_N)_\kappa (d\xi_1^*)_\kappa$$
$$= (d\xi_N^*)_\kappa \prod_{j=2}^{N-1} \left((d\xi_j)_\kappa (d\xi_j^*)_\kappa\right) (d\xi_1)_\kappa (d\xi_N)_\kappa (d\xi_1^*)_\kappa$$
$$= (d\xi_N)_\kappa (d\xi_N^*)_\kappa \prod_{j=2}^{N-1} \left((d\xi_j)_\kappa (d\xi_j^*)_\kappa\right) (d\xi_1)_\kappa (d\xi_1^*)_\kappa = \prod_{j=1}^{N} \left((d\xi_j)_\kappa (d\xi_j^*)_\kappa\right) \ . \quad (3.261)$$

(Note that the 'factors' in parentheses after the product symbols $\prod$ are even and therefore 'commute' with each other.)

The next step we take in calculating the value of the generating functional is to reexponentiate, i. e., to replace

$$\left(\mathbf{1} - \frac{1}{N} H_\kappa(\xi_j^*, \xi_j)\right) \sim e^{-\frac{1}{N} H_\kappa(\xi_j^*, \xi_j)} \quad (3.262)$$

in the above formulas. It is by no means trivial to justify this manipulation. In Appendix C.2 we prove that this is indeed possible, slightly extending an argument given by Salmhofer in [30]. We have thus proved the lemma:

**Lemma 3.41.** *Assume that a selfadjoint, nonnegative operator $H$ in $\mathcal{F}_-$ obeys* (3.232)*. Then we have, for any $\kappa \in \mathbb{N}$,*

$$\sum_{\underline{m},\underline{n} \in \{0,1\}^\kappa} (\eta)_\kappa^{\underline{m}} (\eta^*)_\kappa^{\underline{n}} \operatorname{tr}\left((a)_\kappa^{\underline{n}} (a^*)_\kappa^{\underline{m}} P_\kappa e^{-H} P_\kappa\right)$$
$$= \lim_{N\to\infty} \int \exp\left[\sum_{l,l'=1}^{N} Q_{l,l'} (\xi_l^*)_\kappa \cdot (\xi_{l'})_\kappa\right] \exp\left( - (\eta^*)_\kappa \cdot (\xi_N)_\kappa - (\xi_1^*)_\kappa \cdot (\eta)_\kappa \right)$$
$$\exp\left( -\frac{1}{N} \sum_{j=1}^{N} H_\kappa(\xi_j^*, \xi_j) \right) \prod_{j=1}^{N} \left((d\xi_j)_\kappa (d\xi_j^*)_\kappa\right) \ . \quad (3.263)$$

We now calculate the generating functional in the particle conserving case:

**Theorem 3.42.** *Suppose $h^* = h \geq 0$ is a one-particle operator in $\mathcal{H}^1$, such that*

$$v_\kappa := \mathrm{span}\{f_1, \ldots, f_\kappa\} \subseteq \mathcal{D}(h) \qquad \text{and} \qquad h v_\kappa \subseteq v_\kappa \quad , \qquad \forall\, \kappa \in \mathbb{N} . \tag{3.264}$$

*Then $H := \mathrm{d}\mathbf{G}(h)$ satisfies (3.232) and we have*

$$\mathcal{G}_{H,\kappa} = \exp\left( \tfrac{1}{2}(\eta^*)_\kappa \cdot (\eta)_\kappa - \sum_{k,k'=1}^{\kappa} \eta^*(f_k) \left( \frac{1}{\mathbf{1} + e^{-m_\kappa}} \right)_{k,k'} \eta(f_{k'}) \right) , \tag{3.265}$$

*where $m_\kappa$ denotes the matrix given by*

$$(m_\kappa)_{i,j} := \langle f_i \,|\, h f_j \rangle \quad , \qquad \forall\, i,j \in \{1, \ldots, \kappa\} . \tag{3.266}$$

*Proof:* Clearly, $H$ satisfies the hypothesis of Lemma 3.41 and

$$H_\kappa(\xi_j^*, \xi_j) = \sum_{k,k'=1}^{\kappa} \xi_j^*(f_k)(m_\kappa)_{k,k'} \xi_j(f_{k'}) \quad , \qquad \forall\, j \in \{1, \ldots, N\} . \tag{3.267}$$

We can absorb the matrix $m_\kappa$ into the covariance $Q$ appearing in (3.263) by setting

$$\hat{Q}_{l,k;l',k'} := Q_{l,l'} \delta_{k,k'} + \delta_{l,l'} \left( -\tfrac{1}{N} m_\kappa \right)_{k,k'} \quad , \qquad \forall\, l, l \in \{1, \ldots, N\},\ k, k' \in \{1, \ldots, \kappa\} , \tag{3.268}$$

i. e., as a block matrix,

$$\hat{Q} = \begin{pmatrix} \mathbf{1}_\kappa - \frac{1}{N} m_\kappa & & & \mathbf{1}_\kappa \\ -\mathbf{1}_\kappa & \ddots & & \\ & \ddots & \ddots & \\ & & -\mathbf{1}_\kappa & \mathbf{1}_\kappa - \frac{1}{N} m_\kappa \end{pmatrix} . \tag{3.269}$$

The statement of Lemma 3.41 then reads

$$\begin{aligned} \sum_{\underline{m},\underline{n} \in \{0,1\}^\kappa} & (\eta)_\kappa^{\underline{m}} (\eta^*)_\kappa^{\underline{n}} \operatorname{tr}\left( (a)_\kappa^{\underline{n}} (a^*)_\kappa^{\underline{m}} P_\kappa e^{-H} P_\kappa \right) \\ &= \lim_{N \to \infty} \int \exp\left[ \sum_{l,l'=1}^{N} \sum_{k,k'=1}^{\kappa} \hat{Q}_{l,k;l',k'} \xi_l^*(f_k) \xi_{l'}(f_{k'}) \right] \\ &\qquad \cdot \exp\Big( - (\eta^*)_\kappa \cdot (\xi_N)_\kappa - (\xi_1^*)_\kappa \cdot (\eta)_\kappa \Big) \prod_{j=1}^{N} (d\xi_j)_\kappa (d\xi_j^*)_\kappa . \end{aligned} \tag{3.270}$$

The matrix $\hat{Q}$ is invertible, by the following inversion formula for $N \times N$ block matrices, made up of quadratic blocks $b$, $\mathbf{1}$ and $\mathbf{0}$, all of the size $\kappa \times \kappa$:

$$\begin{pmatrix} b & & & \mathbf{1} \\ -\mathbf{1} & \ddots & & \\ & \ddots & \ddots & \\ & & -\mathbf{1} & b \end{pmatrix}^{-1} = \frac{1}{\mathbf{1} + b^N} \begin{pmatrix} b^{N-1} & -b^0 & \cdots & -b^{N-2} \\ \vdots & b^{N-1} & \cdots & -b^{N-3} \\ \vdots & \vdots & & \vdots \\ \vdots & \vdots & & -b^0 \\ b^0 & b^1 & \cdots & b^{N-1} \end{pmatrix} , \tag{3.271}$$

if only the matrix $\mathbf{1} + b^N$ is invertible. (The 'factor' $(1 + b^N)^{-1}$ on the right hand side is understood to multiply all the blocks in the matrix to its right.) Substituting in (3.270) according to

$$\xi_l^*(f_k) \mapsto \xi_l^*(f_k) - \sum_{k'=1}^{\kappa} \eta^*(f_{k'}) \hat{Q}^{-1}_{N,k';l,k} \qquad \text{and} \qquad \xi_l(f_k) \mapsto \xi_l(f_k) - \sum_{k'=1}^{\kappa} \hat{Q}^{-1}_{l,k;1,k'} \eta(f_{k'}) \ , \tag{3.272}$$

for all $l \in \{1, \dots, N\}$ and $k \in \{1, \dots, \kappa\}$, we obtain

$$\begin{aligned} &\sum_{\underline{m},\underline{n} \in \{0,1\}^\kappa} (\eta)^{\underline{m}}_\kappa (\eta^*)^{\underline{n}}_\kappa \operatorname{tr}\left((a)^{\underline{n}}_\kappa (a^*)^{\underline{m}}_\kappa P_\kappa e^{-H} P_\kappa\right) \\ &\qquad = \lim_{N \to \infty} \exp\left[\sum_{k,k'=1}^{\kappa} \left(\frac{1}{\mathbf{1} + \left(\mathbf{1} - \frac{1}{N} m_\kappa\right)^N}\right)_{k,k'} \eta^*(f_k)\eta(f_{k'})\right] \\ &\qquad\qquad \cdot \int \exp\left[\sum_{l,l'=1}^{N} \sum_{k,k'=1}^{\kappa} \hat{Q}_{l,k;l',k'} \xi_l^*(f_k) \xi_{l'}(f_{k'})\right] \prod_{j=1}^{N} (d\xi_j)_\kappa (d\xi_j^*)_\kappa \ . \end{aligned} \tag{3.273}$$

We note that that the integral on the right hand side is just the partition function (with cut-off). Therefore, we have

$$\begin{aligned} &\sum_{\underline{m},\underline{n} \in \{0,1\}^\kappa} (\eta)^{\underline{m}}_\kappa (\eta^*)^{\underline{n}}_\kappa \operatorname{tr}\left((a)^{\underline{n}}_\kappa (a^*)^{\underline{m}}_\kappa P_\kappa e^{-H} P_\kappa\right) \\ &\qquad = \operatorname{tr}\left(P_\kappa e^{-H}\right) \lim_{N \to \infty} \exp\left(\sum_{k,k'=1}^{\kappa} \eta^*(f_k) \left(\frac{1}{\mathbf{1} + (\mathbf{1} - \frac{1}{N} m_\kappa)^N}\right)_{k,k'} \eta(f_{k'})\right) \\ &\qquad = \operatorname{tr}\left(P_\kappa e^{-H}\right) \exp\left(\sum_{k,k'=1}^{\kappa} \eta^*(f_k) \left(\frac{1}{\mathbf{1} + e^{-m_\kappa}}\right)_{k,k'} \eta(f_{k'})\right) \end{aligned} \tag{3.274}$$

This, together with (3.220), completes our proof. □

**Remark 3.43:** We now generalize Theorem 3.42 to the situation, in which the Hamiltionian is quadratic, but does not necessarily conserve the number of particles. For simplicity we shall assume, for the rest of this subsection, that the one-particle space $\mathcal{H}^1$ is finite dimensional and set $\kappa = \dim \mathcal{H}^1$. We shall use the following statement, the proof of which we shall only sketch (later indicating how this can be made rigorous): For any linear functional $\omega$ on the CAR Algebra and any homogenous Bogoliubov transformation $\tilde{w}$ of the form

$$\tilde{w} = \begin{pmatrix} X^* & Y^T \\ Y^* & X^T \end{pmatrix} \ , \tag{3.275}$$

denoting the associated algebra-automorphism by $\alpha$, we have

$$\begin{aligned} &e^{\frac{1}{2}(\eta^*)_\kappa \cdot (\eta)_\kappa} \sum_{\underline{m},\underline{n} \in \{0,1\}^\kappa} (\eta)^{\underline{m}}_\kappa (\eta^*)^{\underline{n}}_\kappa \omega\Big(\alpha\big((a)^{\underline{n}}_\kappa (a^*)^{\underline{m}}_\kappa\big)\Big) \\ &\qquad = e^{\frac{1}{2}(\tilde{\eta}^*)_\kappa \cdot (\tilde{\eta})_\kappa} \sum_{\underline{m},\underline{n} \in \{0,1\}^\kappa} (\tilde{\eta})^{\underline{m}}_\kappa (\tilde{\eta}^*)^{\underline{n}}_\kappa \omega\big((a)^{\underline{n}}_\kappa (a^*)^{\underline{m}}_\kappa\big) \ , \end{aligned} \tag{3.276}$$

where we have defined new Grassmann variables $\tilde{\eta}$ and $\tilde{\eta}^*$ by

$$\tilde{\eta}^*(f) := \eta^*(Xf)+\eta(Yf) \qquad \text{and} \qquad \tilde{\eta}(f) := \eta(Xf)+\eta^*(Yf) \quad , \qquad \forall\, f \in \mathcal{H}^1 \ . \tag{3.277}$$

The sketchy bit of the proof we shall present is the fact that we do not prove exactly (3.276). Instead we prove the following identity in the Grassmann extended CAR Algebra over $\mathcal{H}^1$ (see Subsection C.3):

$$\begin{aligned} &e^{\frac{1}{2}(\eta^*)_\kappa \cdot (\eta)_\kappa} \sum_{\underline{m},\underline{n} \in \{0,1\}^\kappa} (\eta)^{\underline{m}}_\kappa (\eta^*)^{\underline{n}}_\kappa \alpha\big((a)^{\underline{n}}_\kappa\big) \alpha\big((a^*)^{\underline{m}}_\kappa\big) \\ &\qquad\qquad = e^{\frac{1}{2}(\tilde{\eta}^*)_\kappa \cdot (\tilde{\eta})_\kappa} \sum_{\underline{m},\underline{n} \in \{0,1\}^\kappa} (\tilde{\eta})^{\underline{m}}_\kappa (\tilde{\eta}^*)^{\underline{n}}_\kappa (a)^{\underline{n}}_\kappa (a^*)^{\underline{m}}_\kappa \ , \end{aligned} \tag{3.278}$$

i. e., we pretend that we can pull the Grassmann variables into the argument of the functional $\omega$.

*Proof of (3.278):* Note that the left hand side (l. h. s.) of relation (3.278) is given by

$$\text{l. h. s.} = \exp\left( \sum_{k=1}^{\kappa} \Big( \eta(f_k)\alpha\big(a^*(f_k)\big) + \eta^*(f_k)\alpha\big(a(f_k)\big) \Big) \right) \tag{3.279}$$

by the Baker-Cambell-Hausdorff Relation (here we use the fact that $\alpha(a(\cdot))$ and $\alpha(a^*(\cdot))$ also satisfy the CAR). Now note that

$$\begin{aligned} &\sum_{k=1}^{\kappa} \Big( \eta^*(f_k)\alpha\big(a(f_k)\big) + \eta(f_k)\alpha\big(a^*(f_k)\big) \Big) \\ &\quad = \sum_{k=1}^{\kappa} \Big( \eta^*(f_k)\big(a(X^*f_k) + a^*(Y^T\bar{f}_k)\big) + \eta(f_k)\big(a^*(X^*f_k) + a(Y^T\bar{f}_k)\big) \Big) \\ &\quad = \sum_{k=1}^{\kappa} \big( \tilde{\eta}^*(f_k)a(f_k) + \tilde{\eta}(f_k)a^*(f_k) \big) \ , \end{aligned} \tag{3.280}$$

where we have additionally assumed that the orthonormal one-particle basis $\{f_j\}_{j\in\{1,\ldots,\kappa\}}$ is chosen such that $\bar{f}_j = f_j$, for all $j \in \{1,\ldots,\kappa\}$. From this we obtain, using again the Baker-Cambell-Hausdorff Relation

$$\text{l. h. s.} = \exp\left( \sum_{k=1}^{\kappa} \big( \tilde{\eta}^*(f_k)a(f_k) + \tilde{\eta}(f_k)a^*(f_k) \big) \right) = \text{r. h. s.} \ , \tag{3.281}$$

where we have used the fact that $\tilde{\eta}$ and $\tilde{\eta}^*$ obey the same anti-commutation relations among themselves and with $a$ and $a^*$ as the original Grassmann variables $\eta$ and $\eta^*$. This completes the proof. $\square$

By the linearity of $\omega$, it should be possible to prove (3.276) along the same lines, if one extends the functional $\omega$ to the Grassmann extended CAR Algebra, such that any Grassmann variables may be pulled out to the left. Quite clearly, in the above proof, the fact that $\eta$, $\eta^*$ and $a$, $a^*$ appear as anti-commuting elements of *one* algebra is inessential, since the Baker-Cambell-Hausdorff Relation is used once in one direction and then used again in the other direction. To verify (3.276) directly, however, seems to be combinatorially difficult.

As we have already pointed out, the new Grassmann variables $\tilde{\eta}$ and $\tilde{\eta}^*$ behave exactly in the same way as the original ones[8] $\eta$ and $\eta^*$. It is thus clear from Theorem 3.42 and from identity (3.276) that we have

$$\mathcal{G}_{U_w\, \mathrm{d}\mathbf{G}(h) U_w^*, \kappa} = \exp\Big( \frac{1}{2} (\tilde{\eta}^*)_\kappa \cdot (\tilde{\eta})_\kappa - \sum_{k,k'=1}^{\kappa} \tilde{\eta}^*(f_k) \Big( \frac{1}{\mathbf{1} + e^{-m}} \Big)_{k,k'} \tilde{\eta}(f_k) \Big) \ , \tag{3.283}$$

where we denote by $U_w$ the unitary implementation of the Bogoliubov transformation $w = \tilde{w}^{-1}$.

Now assume that we are given an orthonormal basis $\{f_k\}_{k \in L_+}$ in $\mathcal{L}_+ \cong \mathcal{H}^1$, such that $\bar{f}_k = f_k$, for all $k \in L_+$. For any $k \in L_+ = \{1, \ldots, \kappa\}$, we set $f_{-k} := \tau f_k$ and denote by $L_-$ the family of indices $\{-k \mid k \in L_+\}$ by $L_-$. By the compatibility condition (1.82) it is clear that $\{f_k\}_{k \in L}$ with $L := L_+ \cup L_-$ is an orthonormal basis in $\mathcal{L}$. Since we want to use this basis to represent linear mappings in $\mathcal{L}$ by quadratic matrices, we must choose an ordering of $L$. We choose the following, somewhat unconventional, ordering:

$$L = \{1; \ldots; \kappa; -1; \ldots; -\kappa\} \ , \tag{3.284}$$

the semicolons indicating that $L$ is to be understood as an *ordered* set.

Consider then a quadratic selfadjoint operator $H$ of the form

$$H = \sum_{k,k' \in L} \langle f_k \,|\, M f_{k'} \rangle \, B(f_k) B^*(f_{k'}) \ . \tag{3.285}$$

**Theorem 3.44.** *Let $w$ be a homogeneous Bogoliubov transformation with unitary implementation $U_w$ and such that*

$$H = U_w \, \mathrm{d}\mathbf{G}(h) U_w^* + c \cdot \mathbf{1} \ , \tag{3.286}$$

*for some selfadjoint, nonnegative one-particle operator $h$ in $\mathcal{H}^1$ and some constant $c$. Represent the operator $M$ in* (3.285) *as a matrix with respect to the basis $\{f_k\}_{k \in L}$ and introduce the following row and column vectors of Grassmann variables:*

$$(\eta^*, \eta) := \big( \eta^*(f_1), \ldots, \eta(f_\kappa)^*, \eta(f_1), \ldots, \eta(f_\kappa) \big) \qquad \text{and} \qquad \begin{pmatrix} \eta \\ \eta^* \end{pmatrix} := \begin{pmatrix} \eta(f_1) \\ \vdots \\ \eta(f_\kappa) \\ \eta^*(f_1) \\ \vdots \\ \eta^*(f_\kappa) \end{pmatrix} . \tag{3.287}$$

[8]The careful reader might object that even if $f$ and $g$ are orthogonal to each other, it may still occur that $\tilde{\eta}(f)$ and $\tilde{\eta}(g)$ are linearly dependent and hence their product may evaluate to zero. As a matter of fact, this possibility is not excluded! This is, however, of no relevance to our arguments, since we have repeatedly used the statement

$$f, g \text{ linearly dependent} \quad \Rightarrow \quad \eta(f)\eta(g) = \eta^*(f)\eta^*(g) = 0 \quad , \qquad \forall\, f, g \in \mathcal{H}^1 \ , \tag{3.282}$$

but at no point of the argument, however, we have used the converse implication.

*Using the rules of matrix multiplication, we then have*

$$\mathcal{G}_{H,\kappa} = \exp\left( (\eta^*, \eta) \left( \frac{1}{\mathbf{1} + e^{-M}} \right) \begin{pmatrix} \eta \\ \eta^* \end{pmatrix} \right) \ . \tag{3.288}$$

*Proof:* Let $w$ be of the form

$$w = \begin{pmatrix} X & Y \\ \bar{Y} & \bar{X} \end{pmatrix} \ , \tag{3.289}$$

i. e., $w = \tilde{w}^{-1}$, and denote by $(\tilde{\eta}^*, \tilde{\eta})$ the analogous row vector to $(\eta^*, \eta)$ and correspondingly the column vector. Note that we have

$$\frac{1}{1 + e^{-\tilde{M}}} = \begin{pmatrix} \frac{1}{1-e^{-m}} & \mathbf{0} \\ \mathbf{0} & 2 \cdot \mathbf{1} \end{pmatrix} \qquad \text{with} \qquad \tilde{M} = \begin{pmatrix} m & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix} \ . \tag{3.290}$$

Therefore, we may cast (3.283) into the following shape:

$$\mathcal{G}_{H,\kappa} = \exp\left( -(\tilde{\eta}^*, \tilde{\eta}) \left( \frac{1}{\mathbf{1} + e^{-\tilde{M}}} \right) \begin{pmatrix} \tilde{\eta} \\ \tilde{\eta}^* \end{pmatrix} \right) \ , \tag{3.291}$$

where $m$ is the matrix given by

$$m_{k,k'} := \langle f_k \,|\, h f_{k'} \rangle \quad , \qquad \forall\ k, k' \in \{1, \ldots, \kappa\} \ . \tag{3.292}$$

Next, we note that, using the definition of $\tilde{\eta}$ and $\tilde{\eta}^*$, we have

$$(\tilde{\eta}^*, \tilde{\eta}) = (\eta^*, \eta) w \qquad \text{and} \qquad \begin{pmatrix} \tilde{\eta} \\ \tilde{\eta}^* \end{pmatrix} = w^* \begin{pmatrix} \eta \\ \eta^* \end{pmatrix} \ , \tag{3.293}$$

regarding $X$ and $Y$ as quadratic matrices with respect to the one-particle basis $\{f_1, \ldots, f_\kappa\}$ and also regarding $w$ as a matrix in the same fashion as $M$. This leads us to the conclusion that

$$\mathcal{G}_{H,\kappa} = \exp\left( -(\eta^*, \eta) \left( \frac{1}{\mathbf{1} + e^{-w\tilde{M}w^*}} \right) \begin{pmatrix} \eta \\ \eta^* \end{pmatrix} \right) \ . \tag{3.294}$$

This proves the claim since $w\tilde{M}w^* = M$. $\square$

# Chapter 4

# Hartree-Fock-Bogoliubov-Theory

In this chapter we give a short introduction to what we call Hartree-Fock-Bogoliubov Theory (HFB-Theory), which is also known as Generalized Hartree-Fock Theory. We first sketch the main ideas: The goal is to obtain information on the ground state energy

$$E_0 := \left\{ \omega(H) \;\middle|\; \omega \text{ state} \right\} \tag{4.1}$$

of a many-fermion or a many-boson system, represented by the Hamiltonian $H$. Since this quantity is in most of the cases inaccessible to direct computation, we approximate $E_0$ by the HFB-Energy, denoted by $E_{HFB}$, as follows:

$$E_0 \leq E_{HFB} := \inf\left\{ \omega(H) \;\middle|\; \omega \text{ admissible, quasi-free state} \right\} . \tag{4.2}$$

From a physicist's point of view, this is motivated by the fact that the set of quasi-free states may be interpreted as the set of those states bearing no correlations, except for those imposed by the statistics of the particles. This is reflected by the defining property that all higher truncated functionals of such states vanish (see Theorem 3.2 and Definition 3.24). From a technical point of view, the quantity $E_{HFB}$ is easier to access because the expectation $\omega(H)$, for any quasi-free $\omega$, is expressible entirely in terms of the one-point and the two-point functions of $\omega$ given by

$$\omega\big(a^*(\cdot)a(\cdot)\big) \quad , \quad \omega\big(a^*(\cdot)a^*(\cdot)\big) \quad , \quad \omega\big(a^*(\cdot)\big) \quad , \tag{4.3}$$

for any $H$ polynomial in the creation and annihilation operators. (In the fermionic case, we assume that the states $\omega$ are even, and then the one-point function drops out from our considerations.) That way, we can characterize the HFB-Energy by a variational principle on the convex set of admissible generalized density matrices, see Definition 3.26, or of admissible pairs, see Definition 3.15. In particular, we are interested in the case, in which the one-particle space is given by

$$\mathcal{H}^1 = L^2(\Lambda) \ , \quad \text{with} \qquad \Lambda := (\mathbb{R}/L\mathbb{Z})^3 \ , \tag{4.4}$$

for some size parameter $L > 0$. Furthermore, denote by $\psi \mapsto \bar{\psi}$ the pointwise conjugation of the function $\psi \in L^2(\Lambda)$. The Hamiltonian $H$ is supposed to be of the form

$$H{\restriction}_{\mathcal{H}^1} = \mathrm{d}\mathbf{G}_1(h) \qquad \text{and} \qquad H{\restriction}_{\mathcal{H}^n} = \mathrm{d}\mathbf{G}_n(h) + \lambda V_n \quad , \qquad \forall\, n \in \{2,3,\dots\} \ , \tag{4.5}$$

for some selfadjoint, nonnegative one-particle operator $h$ in $\mathcal{H}^1$ and some coupling parameter $\lambda > 0$. Here, $\mathcal{H}^n$ denotes either the bosonic or the fermionic $n$-particle space. $V_n$ is given by

$$V_n \psi(x_1, \ldots, x_n) := \sum_{1 \leq i < j \leq n} v(x_i - x_j) \psi(x_1, \ldots, x_n) \quad , \qquad \forall\, n \in \{2, 3, \ldots, \} \ , \tag{4.6}$$

with

$$\psi \in \mathcal{D}(V_n) := \left\{ \psi \in L^2\left(\Lambda^n\right) \mid V_n \psi \in L^2\left(\Lambda^n\right) \right\} \ , \tag{4.7}$$

for some nonnegative pair-potential $v$. Here we have used the unitary equivalence

$$\mathcal{H}^n = L^2\left(\Lambda\right)^{\otimes n} \cong L^2\left(\Lambda^n\right) \ , \tag{4.8}$$

and we have denoted by $x_1, \ldots, x_n$ the variables corresponding to the $n$ copies of $\Lambda$. We shall draw no notational distinction between the operators $V_n$ acting in each of these two spaces (and in fact in $\mathcal{H}^n_-$ and $\mathcal{H}^n_+$). Formally, we may write

$$H = \sum_{j, j' \in \mathbb{N}} h_{j,j'} a_j^* a_{j'} + \frac{\lambda}{2} \sum_{j, j', k, k' \in \mathbb{N}} V_{j,j';k,k'} a_{j'}^* a_j^* a_k a_{k'} \ , \tag{4.9}$$

where we have abbreviated

$$h_{j,j'} := \left\langle f_j \,\middle|\, h f_{j'} \right\rangle \quad , \qquad V_{j,j';k,k'} := \left\langle f_j \otimes f_{j'} \,\middle|\, V_2\, f_k \otimes f_{k'} \right\rangle \ , \tag{4.10}$$

and

$$a_j^\sigma := a^\sigma(f_j) \quad , \qquad \forall\, \sigma \in \{\varnothing, *\}, \ j \in \mathbb{N} \ , \tag{4.11}$$

for a suitable orthonormal basis $\{f_j\}_{j \in \mathbb{N}}$ in the one-particle space $\mathcal{H}^1$.

Before we rigorously define the variational principle (4.2) in Subsections 4.2.1 and 4.2.2, it is convenient to introduce a tool, which we discuss in the next subsection.

## 4.1 Decomposition of Radial Pair-Potentials

### 4.1.1 Pair-Potentials on $\mathbb{R}^3$

The notion of a pair-potential has been used in (4.6) without prior explanation. Let us now clarify this. Any measurable function

$$v : \mathbb{R}^3 \setminus \{0\} \to \mathbb{R} \ , \qquad \text{with} \qquad v(x) = v(-x) \quad , \qquad \forall\, x \in \mathbb{R}^3 \setminus \{0\} \ , \tag{4.12}$$

is called a pair-potential on $\mathbb{R}^3$. If, additionally, there exists a function $u : \mathbb{R}^+ \to \mathbb{R}$ such that

$$v(x) = u(|\, x \,|) \quad , \qquad \forall\, x \in \mathbb{R}^3 \setminus \{0\} \ , \tag{4.13}$$

we say that $v$ is a radial pair-potential. We shall exclusively consider radial pair-potentials.

In 1986 Fefferman and de la Llave observed in [15] that the Coulomb potential admits the following representation

$$\frac{1}{|\, x - y \,|} = \frac{1}{\pi} \int_0^\infty dr \frac{1}{r^5} \int_{\mathbb{R}^3} d^3 z\, \chi_r(x - z)\, \chi_r(y - z) \quad , \qquad \forall\, x, y \in \mathbb{R}^3, \ x \neq y \ , \tag{4.14}$$

where we have denoted by $\chi_r$ the characteristic function of the solid ball of radius $r > 0$ centered at the origin. This formula can, except for the normalizing factor, easily be verified, by observing that both sides are homogeneous functions of degree $-1$. Quite obviously, a large class of radial pair-potentials $v$ may be decomposed analogously to (4.14), if the weight function $r \mapsto r^{-5}$ is replaced by a more general one, i. e., if

$$v(x-y) = \int_0^\infty dr\, g(r) \int_{\mathbb{R}^3} d^3z\, \chi_r(x-z)\, \chi_r(y-z) \quad , \qquad \forall\, x, y \in \mathbb{R}^3,\ x \neq y\ , \tag{4.15}$$

for some $g : \mathbb{R}^+ \to \mathbb{R}$. In fact Hainzl and Seiringer in [20] recently gave an inversion formula: They provide a formula for the <u>weight function</u> $g$ in terms of the derivatives of the function $u$ associated to a radial pair-potential $v(\cdot) = u(|\cdot|)$. Another direction into which (4.14) and (4.15) may be generalized is to allow <u>localization functions</u> $d_r$ others than $\chi_r$, such that

$$v(x-y) = \int_0^\infty dr\, g(r) \int_{\mathbb{R}^3} d^3z\, d_r(x-z)\, d_r(y-z) \quad , \qquad \forall\, x, y \in \mathbb{R}^3,\ x \neq y\ . \tag{4.16}$$

We assume the localization functions to be of the form

$$d_r(x) = d\left(\frac{x}{r}\right) \quad , \qquad \forall\, x \in \mathbb{R}^3,\ r > 0\ , \tag{4.17}$$

for some real, essentially bounded, nonnegative and measurable function $d$. Furthermore, the weight function $g$ is assumed to be nonnegative, aswell. For instance, we may use Gaussian localization functions by setting:

$$d(x) := e^{-|x|^2} \quad , \qquad \forall\, x \in \mathbb{R}^3\ . \tag{4.18}$$

As the following theorem shows, the corresponding inversion formula is, in this case, related to the well-known Laplace transformation.

**Theorem 4.1.** *Let $v : \mathbb{R}^3 \setminus \{0\} \to \mathbb{R}$ be a radial pair-potential with $v(\cdot) = u(|\cdot|)$, such that*

$$u\big(\sqrt{s}\big) = \int_0^\infty dt\, e^{-ts} h(s) \quad , \qquad \forall\ \in \mathbb{R}^+\ , \tag{4.19}$$

*for some integrable function $h : \mathbb{R}^+ \to \mathbb{R}_0^+$. We then have*

$$v(x-y) = \int_0^\infty dr \frac{\kappa(r)}{r^5} \int d^3z\ \exp\left(-\frac{1}{r^2}|x-z|^2 - \frac{1}{r^2}|y-z|^2\right) \tag{4.20}$$

*with*

$$\kappa(r) = \left(\frac{2}{\pi}\right)^{\frac{3}{2}} \frac{1}{r} h\left(\frac{1}{2r^2}\right) \quad , \qquad \forall\, r \in \mathbb{R}^+\ . \tag{4.21}$$

Note that we have simply *assumed* the existence of a function $h$ such that (4.19) holds.

*Proof of Theorem 4.1:* We would like to determine $\kappa$ in such a way that

$$v(x) = \int_0^\infty dr\, \frac{\kappa(r)}{r^5} \int_{\mathbb{R}^3} d^3z\ \exp\left(-\frac{1}{r^2}|x-z|^2 - \frac{1}{r^2}|z|^2\right) \quad , \qquad \forall\, x \in \mathbb{R}^3 \setminus \{0\}\ . \tag{4.22}$$

The inner integration can be carried out after completing the square in the exponential. Therefore (4.22) is equivalent to

$$v(x) = \frac{\pi^{\frac{3}{2}}}{4} \int_0^\infty dr\, \kappa\Big((2r)^{-\frac{1}{2}}\Big) r^{-\frac{1}{2}} e^{-|\,x\,|^2 r} \quad , \qquad \forall\, x \in \mathbb{R}^3 \setminus \{0\} \ . \tag{4.23}$$

This is in turn equivalent to

$$u\big(\sqrt{s}\big) = \int_0^\infty dr\, h(r) e^{-sr} \qquad \text{with} \qquad h(r) := \frac{\pi^{\frac{3}{2}}}{4} \kappa\Big((2r)^{-\frac{1}{2}}\Big) \frac{1}{\sqrt{r}} \ , \tag{4.24}$$

for all $s, r > 0$. Solving the last expression for $\kappa$, we obtain (4.21). □

We can use the above theorem to decompose the Coulomb Potential in terms of Gaussian localization functions,

$$\frac{1}{|\,x-y\,|} = \frac{4}{\pi^2} \int_0^\infty dr\, \frac{1}{r^5} \int_{\mathbb{R}^3} d^3z\, \exp\left(-\frac{1}{r^2}|\,x-z\,|^2 - \frac{1}{r^2}|\,y-z\,|^2\right) \ , \tag{4.25a}$$

or to decompose the Yukawa Potential

$$\frac{e^{-\nu|\,x-y\,|}}{|\,x-y\,|} = \frac{4}{\pi^2} \int_0^\infty dr\, \frac{e^{-\frac{1}{2}\nu^2 r^2}}{r^5} \int_{\mathbb{R}^3} d^3z\, \exp\left(-\frac{1}{r^2}|\,x-z\,|^2 - \frac{1}{r^2}|\,y-z\,|^2\right) \ , \tag{4.25b}$$

for all real $x \neq y$ in $\mathbb{R}^3$ and some $\nu \geq 0$. The formulas concerning Laplace transforms, necessary to verify (4.25a) and (4.25b) may be found in [1]. Before we close this section, let us remark that, if the pair-potential $v$ admits a decomposition of the type (4.16), we shall write the operator $V_2$ in the following way:

$$V_2 = \int_0^\infty dr\, g(r) \int_{\mathbb{R}^3} d^3z\, D_{r,z}^2 \otimes D_{r,z}^2 \tag{4.26}$$

with

$$D_{r,z}\psi(x) := d_r(x-z)^{\frac{1}{2}} \psi(x) \quad , \qquad \forall\, x \in \mathbb{R}^3,\ \psi \in \mathcal{H}^1 \ . \tag{4.27}$$

### 4.1.2 Pair-Potentials on $(\mathbb{R}/L\mathbb{Z})^3$

We shall now see how the decomposition formulas of the last section carry over to pair-potentials on the torus $\Lambda = (\mathbb{R}/L\mathbb{Z})^3$, for any $L > 0$. The notion of a pair-potential on the torus is defined in a manner completely analogous to a pair-potential on $\mathbb{R}^3$. The pair-potentials and localization functions on $\mathbb{R}^3$ of the last section will be denoted by $\tilde{v}$ and $\tilde{d}_r$, respectively, those on the torus by $v$ and $d_r$, respectively.

**Definition 4.2.** *A pair-potential $\tilde{v}$ on $\mathbb{R}^3$ is called summable if for any $L' > 0$, we have*

$$\sum_{l \in (L'\mathbb{Z})^3} |\,\tilde{v}(x+l)\,| < \infty \quad , \qquad \forall\, x \in (0, L')^3 \ . \tag{4.28}$$

Obviously the Yukawa Potential (4.25b) is summable, while the Coulomb Potential is not. To any summable pair-potential $\tilde{v}$, we may associate a pair-potential $v$ on $\Lambda$ simply by setting:

$$v(x-y) := \sum_{l \in (L\mathbb{Z})^3} \tilde{v}(x-y+l) \quad , \qquad \forall\, x,y \in \Lambda,\ x \neq y\ . \tag{4.29}$$

Supposing that $\tilde{v}$ has a decomposition of the type (4.16) with weight function $g$ and localization functions $\tilde{d}_r$, we obtain

$$\begin{aligned} v(x-y) &= \sum_{l \in (L\mathbb{Z})^3} \int_0^\infty dr\, g(r) \int_{\mathbb{R}^3} d^3z\, \tilde{d}_r(x+l-z)\, \tilde{d}_r(y-z) \\ &= \int_0^\infty dr\, g(r) \int_\Lambda d^3z \sum_{l,l' \in (L\mathbb{Z})^3} \tilde{d}_r(x+l-z-l')\, \tilde{d}_r(y-z-l') \\ &= \int_0^\infty dr\, g(r) \int_\Lambda d^3z\, d_r(x-z)\, d_r(y-z)\ , \end{aligned} \tag{4.30}$$

for all $x \neq y$ in $\Lambda$ and with

$$d_r(\cdot) := \sum_{l \in (L\mathbb{Z})^3} \tilde{d}_r(\cdot + l)\ . \tag{4.31}$$

Note that the weight function $g$ is the same for both $v$ and $\tilde{v}$. We recall that $g$ is assumed to be nonnegative. Furthermore, the functions $\tilde{d}_r$ are also assumed to be nonnegative, for all $r > 0$, implying that so are the functions $d_r$, for all $r > 0$.

We shall from now on consider only pair potentials on $\Lambda$ allowing a decomposition of the type

$$v(x-y) = \int_0^\infty dr\, g(r) \int_\Lambda d^3z\, d_r(x-z)\, d_r(y-z) \quad , \qquad \forall\, x,y \in \Lambda,\ x \neq y\ , \tag{4.32}$$

for some family $\{d_r\}_{r>0}$ of nonnegative, bounded and measurable functions $d_r$ on $\Lambda$ and a nonnegative, measurable weight function $g$ on $\mathbb{R}^+$.

Analogously to (4.26), we then write the associated maximal multiplication operator on $L^2(\Lambda)$ as

$$V_2 = \int_0^\infty dr\, g(r) \int_\Lambda d^3z\, D_{r,z}^2 \otimes D_{r,z}^2\ , \tag{4.33}$$

where the bounded, nonnegative operators $D_{r,z}$ in $\mathcal{H}^1$ are given as the everywhere defined multiplication operators associated to the bounded functions $d_r(\cdot - z)^{\frac{1}{2}}$. Note that the norm of $D_{r,z}$ may depend on $r$.

As an example, consider the Yukawa Potential on the torus

$$v_\nu(x-y) := \sum_{l \in (L\mathbb{Z})^3} \frac{e^{-\nu|\,x-y-l\,|}}{|\,x-y-l\,|} \quad , \qquad \forall\, x,y \in \Lambda,\ x \neq y\ , \tag{4.34a}$$

for any $\nu \geq 0$. $v_\nu$ admits, by (4.25b), a decomposition of the form (4.32) with

$$g(r) := \frac{4}{\pi^2} \frac{e^{-\frac{1}{2}r^2\nu^2}}{r^5} \qquad \text{and} \qquad d_r(x) := \sum_{l \in (L\mathbb{Z})^3} \exp\left(-\frac{1}{r^2}(x-l)^2\right)\ , \tag{4.34b}$$

for all $x \in \Lambda$ and all $r \in \mathbb{R}^+$.

## 4.2 The Variational Principle

We shall now associate to the formal expression (4.5) a variational principle on generalized density matrices, corresponding to (4.2). In doing so, however, we avoid to go into the details of how to give a precise operator meaning to $H$. Rather, we shall simply write down an associated variational principle, marking the starting point of HFB-Theory. On a formal level, it is easy to verify that the definitions we make are appropriate.

### 4.2.1 Bosonic Theory

We begin by introducing the notion of bosonic two-particle density matrices. Suppose we are given a quasi-free bosonic state $\omega$. As a consequence of (3.4), we have for any set $\{f_j\}_{j\in\mathbb{N}}$ of vectors in $\mathcal{H}^1$:

$$\omega\big(a^*(f_i)a^*(f_j)a(f_k)a(f_l)\big) \\ = (\alpha^*_\omega)_{j,i}(\alpha_\omega)_{l,k} + (\gamma_\omega)_{k,i}(\gamma_\omega)_{l,j} + (\gamma_\omega)_{l,i}(\gamma_\omega)_{k,j} - 2u_iu_j\bar{u}_k\bar{u}_l \ , \quad (4.35)$$

where we have denoted the matrix elements of the entries of $\Gamma_\omega$ in the following way:

$$(\alpha_\omega)_{i,j} := \langle f_i \,|\, \alpha_\omega f_j\rangle = \omega\big(a(\bar{f}_j)a(f_i)\big) \ , \quad (4.36a)$$

$$(\gamma_\omega)_{i,j} := \langle f_i \,|\, \gamma_\omega f_j\rangle = \omega\big(a^*(f_j)a(f_i)\big) \ , \quad (4.36b)$$

and

$$u_i := u(f_i) \ , \quad \text{with} \qquad v\left(\left(\begin{array}{c} f^+ \\ f^- \end{array}\right)\right) = u(f^+) + \bar{u}(f^-) \quad , \quad \forall\, f^\pm \in \mathcal{H}^1 \ , \quad (4.37)$$

are the values of the one-point functional. As we have pointed out in Remark 3.17, admissibility of $\omega$ entails the trace-class property for $\gamma_\omega$, the Hilbert-Schmidt property for $\alpha_\omega$ and $\sum_i |\,u_i\,|^2 < \infty$. Therefore, (4.35) defines by (4.38) a bounded, nonnegative quadratic form and thus the following definition makes sense.

**Definition 4.3.** *Let $\omega$ be a bosonic state which is admissible and quasi-free. Suppose $\{f_j\}_{j\in\mathbb{N}}$ is an orthonormal basis in $\mathcal{H}^1$. The nonnegative trace-class operator $M_\omega$ in $\mathcal{H}^2$, defined by*

$$\langle f_i \otimes f_j \,|\, M_\omega\, f_k \otimes f_l\rangle = \omega\big(a^*(f_l)a^*(f_k)a(f_i)a(f_j)\big) \quad , \qquad \forall\, i,j,k,l \in \mathbb{N} \ , \quad (4.38)$$

*is called the* <u>*two-particle density matrix*</u> *of $\omega$.*

We now proceed to clarify how we intend to evaluate the expectation value of $H$, defined in (4.5), in the admissible state $\omega$. Note that

$$\omega(H) := \mathrm{tr}(h\,\gamma_\omega) + \frac{\lambda}{2}\,\mathrm{tr}(V_2\,M_\omega) \quad (4.39)$$

is perfectly well-defined, as long as the operators $V_2$ and $h$ are bounded. Formally, one may arrive at this expression, by simply inserting the definition of $H$ and using (4.15). However, if either one of these operators is unbounded, we have yet to make sense of the expressions $\mathrm{tr}(h\gamma_\omega)$ and $\mathrm{tr}(V_2M_\omega)$. This is the content of the following proposition.

**Proposition 4.4.** *Suppose we are given two selfadjoint, nonnegative operators $A$ and $B$ in some complex Hilbert space $\mathcal{H}$. Assume, additionally, that $B$ is trace-class. Then the expression*

$$\mathrm{tr}\left(\mathcal{I}_n(A)B\right) \qquad \text{with} \qquad \mathcal{I}_n(x) := \begin{cases} 0 & \text{if } x \leq 0 \\ x & \text{if } 0 < x \leq n \\ n & \text{if } n < x \end{cases} \quad , \qquad \forall\, x \in \mathbb{R} \ , \tag{4.40}$$

*has a limit in $\mathbb{R}^+ \cup \{+\infty\}$, as $n \to \infty$. Moreover, if $A$ is bounded, this limit coincides with* $\mathrm{tr}(AB)$*.*

*Proof:* For any $n \in \mathbb{N}$, the operator $\mathcal{I}_n(A)$ is bounded and nonnegative. Since $B$ is trace-class, we have

$$t_n := \mathrm{tr}\left(\mathcal{I}_n(A)B\right) = \mathrm{tr}\left(\mathcal{I}_n(A)^{\frac{1}{2}}\, B\, \mathcal{I}_n(A)^{\frac{1}{2}}\right) \geq 0 \quad , \qquad \forall\, n \in \mathbb{N} \ . \tag{4.41}$$

Furthermore, for any $n \in \mathbb{N}$, the operator $\mathcal{I}_{n+1}(A) - \mathcal{I}_n(A)$ is bounded and nonnegative. Thus we also have

$$\begin{aligned} t_{n+1} - t_n &= \mathrm{tr}\left((\mathcal{I}_{n+1}(A) - \mathcal{I}_n(A))B\right) \\ &= \mathrm{tr}\left(\left(\mathcal{I}_{n+1}(A) - \mathcal{I}_n(A)\right)^{\frac{1}{2}} B \left(\mathcal{I}_{n+1}(A) - \mathcal{I}_n(A)\right)^{\frac{1}{2}}\right) \geq 0 \ . \end{aligned} \tag{4.42}$$

Therefore the sequence $\{t_n\}_{n\in\mathbb{N}}$ is positive and monotonically nondecreasing and therefore possesses a limit in $\mathbb{R}^+ \cup \{+\infty\}$. If $A$ is bounded, then, for $n > \|\, A\,\|$, we have

$$t_n = \mathrm{tr}(AB) \ . \tag{4.43}$$

□

Thus by (4.40) we can always make sense of (4.39), by

$$\mathrm{tr}(h\gamma_\omega) := \lim_{n\to\infty} \mathrm{tr}\left(\mathcal{I}_n(h)\gamma_\omega\right) \qquad \text{and} \qquad \mathrm{tr}(V_2 M_\omega) := \lim_{n\to\infty} \mathrm{tr}\left(\mathcal{I}_n(V_2)M_\omega\right) \ . \tag{4.44}$$

The next proposition unfolds the full strength of the decomposition formula for radial pair-potentials discussed in the previous sections.

**Proposition 4.5.** *Let the interaction operator $V_2$ (possibly unbounded) admit a decomposition of the type* (4.33)*. We then have, for any two-particle density matrix $M$ corresponding to an admissible quasi-free state:*

$$\mathrm{tr}(V_2 M) = \int_0^\infty dr\, g(r) \int_\Lambda d^3 z\, \mathrm{tr}\left((D_{r,z}^2 \otimes D_{r,z}^2)M\right) \ . \tag{4.45}$$

As we have already remarked, in our applications the operators $D_{r,z}$ are nonnegative and bounded, for any $r \in \mathbb{R}^+$ and any $z \in \Lambda$. Obviously the same is true for the operators $D_{r,z}^2 \otimes D_{r,z}^2$ and hence the traces on the right hand side of (4.45) do all exist and are finite.

*Proof:* By Proposition 4.4 we may write

$$\mathrm{tr}(V_2 M) = \lim_{n\to\infty} \mathrm{tr}\left(\mathcal{I}_n(V_2)M\right) \ , \tag{4.46}$$

where the $\mathcal{I}_n$ are given in (4.40). Furthermore, we write for all $m \in \mathbb{N}$ and all $x$ and $y$ in $\Lambda$

$$v_m(x-y) := \int_0^m dr\, g(r) \int_\Lambda d^3z\, d_r(x-z) d_r(y-z) \ , \tag{4.47}$$

recalling that the functions $g$ and $d_r$, for all $r > 0$, are assumed to be nonnegative. We observe that the sequence $\{v_m(x-y)\}_{m\in\mathbb{N}}$ is monotonically nondecreasing, for all $x, y \in \Lambda$. By expanding out the trace in an orthonormal basis $\{F_j\}_{j\in\mathbb{N}}$ of eigenvectors of $M$, with corresponding eigenvalues $\{\mu_j\}_{j\in\mathbb{N}}$, we obtain

$$\mathrm{tr}(V_2 M) = \lim_{n\to\infty} \sum_{j\in\mathbb{N}} \mu_j \int_\Lambda d^3x\, d^3y \mid F_j(x,y) \mid^2 \mathcal{I}_n\left(\lim_{m\to\infty} v_m(x-y)\right) \ . \tag{4.48}$$

By the fact that each $\mathcal{I}_n$ is continuous, we may pull out the limit $m \to \infty$ and so obtain

$$\mathrm{tr}(V_2 M) = \lim_{n\to\infty} \lim_{m\to\infty} \sum_{j\in\mathbb{N}} \mu_j \int_\Lambda d^3x\, d^3y \mid F_j(x,y) \mid^2 \mathcal{I}_n\big(v_m(x-y)\big) \ . \tag{4.49}$$

Since the limits in $m$ and $n$ are monotonically nondecreasing, we may interchange them. It therefore holds

$$\mathrm{tr}(V_2 M) = \lim_{m\to\infty} \sum_{j\in\mathbb{N}} \mu_j \int_\Lambda d^3x\, d^3y \mid F_j(x,y) \mid^2 v_m(x-y) \ . \tag{4.50}$$

Note that $v_m$ is a bounded function, for any $m \in \mathbb{N}$, and so the integral on the right hand side always exists. By Fubini's Theorem and by monotone convergence, we also have

$$\begin{aligned} \mathrm{tr}(V_2 M) &= \int_0^\infty dr\, g(r) \int_\Lambda d^3z \sum_{j\in\mathbb{N}} \mu_j \int_\Lambda d^3x\, d^3y \mid F_j(x,y) \mid^2 d_r^2(x-z) d_r^2(y-z) \\ &= \int_0^\infty dr\, g(r) \int_\Lambda \mathrm{tr}\left((D_{r,z}^2 \otimes D_{r,z}^2)M\right) \ . \end{aligned} \tag{4.51}$$

□

Now that we have shown how to make sense of $\omega(H)$ and have got around the problem of computing traces of operators, which may not even be bounded, we can use (4.35) to completely eliminate the two-particle density matrix from our discussion. Namely, we have

$$\begin{aligned} \mathrm{tr}(V_2 M_\omega) = \int_0^\infty dr\, g(r) \int_\Lambda d^3z \Big\{ &\mathrm{tr}\left(D_{r,z}^2 \alpha_\omega^* D_{r,z}^2 \alpha_\omega\right) + \mathrm{tr}\left(D_{r,z}^2 \gamma_\omega D_{r,z}^2 \gamma_\omega\right) \\ &+ \mathrm{tr}\left(D_{r,z}^2 \gamma_\omega\right)^2 - 2\Big(\sum_{p\in\mathbb{N}} \mid u(D_{r,z} f_p) \mid^2\Big)^2 \Big\} \ , \end{aligned} \tag{4.52}$$

for any admissible quasi-free state $\omega$. Finally, we are in the position to reformulate the variational principle (4.2) in the bosonic context in a completely rigorous way, involving an energy functional $\mathcal{E}_H$ depending only on the generalized density matrix and the one-point functional:

$$E_{HFB} := \inf\left\{ \mathcal{E}_H\big((\Gamma, v)\big) \;\Big|\; (\Gamma, v) \text{ admissible pair} \right\} , \tag{4.53}$$

with

$$\mathcal{E}_H\big((\Gamma, v)\big) := \mathrm{tr}(h\gamma) + \frac{\lambda}{2}\int_0^\infty dr\, g(r) \int_\Lambda d^3z \Big\{ \mathrm{tr}(D^2_{r,z}\alpha^* D^2_{r,z}\alpha) + \mathrm{tr}(D^2_{r,z}\gamma D^2_{r,z}\gamma) \\ + \mathrm{tr}(D^2_{r,z}\gamma)^2 - 2\Big(\sum_{p\in\mathbb{N}} |\, u(D_{r,z}f_p)\,|^2\Big)^2 \Big\} , \tag{4.54}$$

where $\alpha$, $\gamma$ and $u$ are defined by:

$$\Gamma = \begin{pmatrix} \gamma & \alpha \\ -\bar{\alpha} & -\mathbf{1} - \bar{\gamma} \end{pmatrix} \qquad \text{and} \qquad v\left(\begin{pmatrix} f_+ \\ f_- \end{pmatrix}\right) = u(f_+) + \bar{u}(f_-) . \tag{4.55}$$

We recall Definition 3.15: If $(\Gamma, v)$ is an admissible pair, then $\gamma$ is trace-class, $\alpha^T = \alpha$, $u$ is continuous and

$$\langle f^+ \,|\, \gamma f^+ \rangle + 2\,\mathrm{Re}\,\langle f^+ \,|\, \alpha f^- \rangle + \langle f^- \,|\, (\mathbf{1}+\gamma) f^- \rangle - \big|\, u(f^+) + \bar{u}(f^-)\,\big|^2 \geq 0 , \tag{4.56}$$

for all $f^\pm \in \mathcal{H}^1$. The last condition is equivalent to (3.66). As we have pointed out in Remark 3.17 the Hilbert-Schmidt condition for $\alpha$ is implied.

### 4.2.2 Fermionic Theory

Again, the first step is to introduce the notion of the two-particle density matrix $M_\omega$ associated to a fermionic state $\omega$. At this point, we may allow ourselves a little bit more of generality as compared to the boson case, due to the fact that the mappings $f \mapsto a^*(f)$ and $f \mapsto a(f)$ are bounded. Therefore, the following definition makes sense without further assumptions on the state $\omega$.

**Definition 4.6.** *Let $\omega$ be a state on the CAR Algebra $\mathcal{A}_{car}(\mathcal{H}^1)$ and suppose $\{f_j\}_{j\in\mathbb{N}}$ is an orthonormal basis in $\mathcal{H}^1$. The following defines a bounded, nonnegative operator $M_\omega$ in $\mathcal{H}^2$*

$$\langle f_i \otimes f_j \,|\, M_\omega\, f_k \otimes f_l \rangle = \omega\big(a^*(f_l)a^*(f_k)a(f_i)a(f_j)\big) \quad , \qquad \forall\; i,j,k,l \in \mathbb{N} , \tag{4.57}$$

*which is called the two-particle density matrix associated to $\omega$.*

In order to write the expectation $\omega(H)$ in a manner similar to (4.39), we must ensure that $M_\omega$ is trace-class. This is where the admissibility condition comes in. Indeed, if $\omega$ is a quasi-free state, we have

$$\langle f_i \otimes f_j \,|\, M_\omega\, f_k \otimes f_l \rangle = (\alpha^*_\omega)_{k,l}(\alpha_\omega)_{j,i} - (\gamma_\omega)_{i,l}(\gamma_\omega)_{j,k} + (\gamma_\omega)_{j,l}(\gamma_\omega)_{i,k} , \tag{4.58}$$

where we have denoted the matrix elements of the entries of $\Gamma_\omega$ by

$$(\alpha_\omega)_{i,j} := \langle f_i \,|\, \alpha_\omega f_j \rangle = \omega\big(a(\bar{f}_j)a(f_i)\big) , \tag{4.59a}$$

$$(\gamma_\omega)_{i,j} := \langle f_i \,|\, \gamma_\omega f_j \rangle = \omega\big(a^*(f_j)a(f_i)\big) . \tag{4.59b}$$

Thus, since we know that the admissibility of $\omega$ entails the trace-class property for $\gamma_\omega$ and the Hilbert-Schmidt property for $\alpha_\omega$, we have:

$$\omega \text{ admissible} \quad \Rightarrow \quad M_\omega \text{ trace-class} . \tag{4.60}$$

Since we are only interested in states $\omega$ which are admissible and quasi-free, we always assume that $M_\omega$ is trace-class. It is therefore clear that

$$\omega(H) := \operatorname{tr}(h\gamma_\omega) + \frac{\lambda}{2} \operatorname{tr}(V_2 M_\omega) \tag{4.61}$$

is perfectly well-defined, as long as $h$ and $V_2$ are bounded operators in $\mathcal{H}^1$ and $\mathcal{H}^2$, respectively. Formally, one may arrive at this expression, by simply inserting the definition of $H$ and using (4.59). Again, if $h$ or $V_2$ are unbounded, we can still make sense of (4.61) by positivity, using Proposition 4.4, i. e.,

$$\operatorname{tr}(h\gamma_\omega) := \lim_{n\to\infty} \operatorname{tr}\left(\mathcal{I}_n(h)\gamma_\omega\right) \qquad \text{and} \qquad \operatorname{tr}(V_2 M_\omega) := \lim_{n\to\infty} \operatorname{tr}\left(\mathcal{I}_n(V_2) M_\omega\right) , \tag{4.62}$$

with

$$\mathcal{I}_n(x) := \begin{cases} 0 & \text{if } x \le 0 \\ x & \text{if } 0 < x \le n \\ n & \text{if } n < x \end{cases} , \qquad \forall\, x \in \mathbb{R},\ n \in \mathbb{N} . \tag{4.63}$$

As we have shown before, these definitions are compatible with the usual ones, if $h$ or $V_2$ are bounded. Similarly to the boson case, we may get rid of the limits in (4.62), by Proposition 4.5. Namely, we have for any interaction operator $V_2$, admitting a decomposition of the type (4.33) and any two-particle density matrix $M$ associated to an admissible state:

$$\operatorname{tr}(V_2 M) = \int_0^\infty dr\, g(r) \int_\Lambda d^3z \operatorname{tr}\left((D^2_{r,z} \otimes D^2_{r,z}) M\right) . \tag{4.64}$$

Note that the operators $(D^2_{r,z} \otimes D^2_{r,z})M$ are trace-class, for all $r > 0$ and all $z \in \Lambda$.

Now that we have shown how to make sense of $\omega(H)$ and have got around the problem of computing traces of operators, which may not even be bounded, we can use (4.58) to completely eliminate the two-particle density matrix from our discussion. Namely, we have

$$\operatorname{tr}(V_2 M_\omega) = \int_0^\infty dr\, g(r) \int_\Lambda d^3z \left\{ \operatorname{tr}(D^2_{r,z}\alpha^*_\omega D^2_{r,z}\alpha_\omega) - \operatorname{tr}(D^2_{r,z}\gamma_\omega D^2_{r,z}\gamma_\omega) + \operatorname{tr}(D^2_{r,z}\gamma_\omega)^2 \right\} . \tag{4.65}$$

Finally, we are now in the position to reformulate the variational principle (4.2) in the fermionic context in a completely rigorous way, in terms of an energy functional $\mathcal{E}_H$, depending only on the generalized density matrix.

$$E_{HFB} := \inf \left\{ \mathcal{E}_H(\Gamma) \;\middle|\; \Gamma \text{ admissible generalized density matrix} \right\} , \tag{4.66}$$

with

$$\begin{aligned} \mathcal{E}_H(\Gamma) &:= \operatorname{tr}(h\gamma) \\ &\quad + \frac{\lambda}{2} \int_0^\infty dr\, g(r) \int_\Lambda d^3z \left\{ \operatorname{tr}(D^2_{r,z}\alpha^* D^2_{r,z}\alpha) - \operatorname{tr}(D^2_{r,z}\gamma D^2_{r,z}\gamma) + \operatorname{tr}(D^2_{r,z}\gamma)^2 \right\} , \end{aligned} \tag{4.67}$$

where $\alpha$ and $\gamma$ are given by

$$\Gamma = \begin{pmatrix} \gamma & \alpha \\ -\bar{\alpha} & 1-\bar{\gamma} \end{pmatrix} . \tag{4.68}$$

We recall that if $\Gamma$ is an admissible generalized density matrix, then $\alpha^T = -\alpha$, $\gamma$ is Hilbert-Schmidt and

$$\langle f^+ \,|\, \gamma f^+ \rangle + 2\,\mathrm{Re}\,\langle f^+ \,|\, \alpha f^- \rangle + \langle f^- \,|\, (\mathbf{1}-\gamma) f^- \rangle \geq 0 , \tag{4.69}$$

for all $f^\pm \in \mathcal{H}^1$. Again, it is implied that $\alpha$ is Hilbert-Schmidt.

### 4.2.3 Self-Consistency

Even though the problem of calculating the HFB-Energy is far less complex than the problem of calculating the ground state Energy $E_0$, it is often still not feasible to determine $E_{HFB}$ rigorously. For the sake of completeness we shortly describe the idea of self-consistency. To this end, let us introduce the following notions. (Lemmas 4.7 and 4.8 will motivate this definitions.)

**Fermionic Self-Consistent Energy Functional:**

$$\begin{aligned}\mathcal{E}_H^{sc}(\Gamma,\tilde{\Gamma}) := {} & \mathrm{tr}(h\gamma) \\ & + \frac{\lambda}{2}\int_0^\infty dr\, g(r) \int_\Lambda d^3z \Big\{ 2\,\mathrm{Re}\,\mathrm{tr}(D_{r,z}^2 \alpha^* D_{r,z}^2 \tilde{\alpha}) - 2\,\mathrm{tr}(D_{r,z}^2 \gamma D_{r,z}^2 \tilde{\gamma}) \\ & \qquad + 2\,\mathrm{tr}(D_{r,z}^2\gamma)\,\mathrm{tr}(D_{r,z}^2\tilde{\gamma}) \Big\} .\end{aligned} \tag{4.70}$$

**Bosonic Self-Consistent Energy Functional:**

$$\begin{aligned}\mathcal{E}_H^{sc}\big((\Gamma,v),(\tilde{\Gamma},\tilde{v})\big) := {} & \mathrm{tr}(h\gamma) \\ + \frac{\lambda}{2}\int_0^\infty dr\, g(r) \int_\Lambda d^3z & \Big\{ 2\,\mathrm{Re}\,\mathrm{tr}(D_{r,z}^2 \alpha^* D_{r,z}^2 \tilde{\alpha}) + 2\,\mathrm{tr}(D_{r,z}^2 \gamma D_{r,z}^2 \tilde{\gamma}) \\ & + 2\,\mathrm{tr}(D_{r,z}^2\gamma)\,\mathrm{tr}(D_{r,z}^2\tilde{\gamma}) \\ & - 8\,\mathrm{Re}\Big(\sum_p |\,\tilde{u}(D_{r,z}f_p)\,|^2\Big) \sum_p \tilde{u}(D_{r,z}f_p)\overline{u(D_{r,z}f_p)} \Big\} .\end{aligned} \tag{4.71}$$

Here, $\gamma$ and $\alpha$ denote the entries of $\Gamma$, $\tilde{\gamma}$ and $\tilde{\alpha}$ denote the entries of $\tilde{\Gamma}$. In the boson case $u$ and $\tilde{u}$ are determined by the one-point functionals $v$ and $\tilde{v}$ via:

$$v\left(\begin{pmatrix} f^+ \\ f^- \end{pmatrix}\right) = u(f^+) + \bar{u}(f^-) \qquad \text{and} \qquad \tilde{v}\left(\begin{pmatrix} f^+ \\ f^- \end{pmatrix}\right) = \tilde{u}(f^+) + \overline{\tilde{u}}(f^-) , \tag{4.72}$$

for all $f^\pm \in \mathcal{H}^1$.

Formally, the functionals (4.70) and (4.71) are the energy expectation values in the state $\omega$ associated to $(\Gamma, v)$ of the following self-consistent Hamiltonians.

**Fermionic Self-Consistent Hamiltonian:**

$$\begin{aligned} H_{\tilde{\omega}} = & \sum_{j,j'} h_{j,j'} a_j^* a_{j'} \\ & + \frac{\lambda}{2} \sum_{j,j',k,k'} V_{j,j';k,k'} \Big\{ \tilde{\omega}(a_k a_{k'}) a_{j'}^* a_j^* + \tilde{\omega}(a_{j'}^* a_j^*) a_k a_{k'} - \tilde{\omega}(a_j^* a_{k'}) a_{j'}^* a_k \\ & - \tilde{\omega}(a_{j'}^* a_k) a_j^* a_{k'} + a_{j'}^* a_{k'} \tilde{\omega}(a_j^* a_k) + \tilde{\omega}(a_{j'}^* a_{k'}) a_j^* a_k \Big\} , \end{aligned} \tag{4.73}$$

where $\tilde{\omega}$ is any state having $\tilde{\Gamma}$ as its generalized density matrix.

**Bosonic Self-Consistent Hamiltonian:**

$$\begin{aligned} H_{\tilde{\omega}} = & \sum_{j,j'} h_{j,j'}\, a_j^* a_{j'} \\ & + \frac{\lambda}{2} \sum_{j,j',k,k'} V_{j,j';k,k'} \Big\{ \tilde{\omega}(a_k a_{k'})\, a_{j'}^* a_j^* + \tilde{\omega}(a_{j'}^* a_j^*)\, a_k a_{k'} + \tilde{\omega}(a_j^* a_{k'})\, a_{j'}^* a_k + \tilde{\omega}(a_{j'}^* a_k)\, a_j^* a_{k'} \\ & + \tilde{\omega}(a_j^* a_k)\, a_{j'}^* a_{k'} + \tilde{\omega}(a_{j'}^* a_{k'})\, a_j^* a_k - 2\tilde{\omega}(a_{j'}^* a_j^* a_k)\, a_{k'} \\ & - 2\tilde{\omega}(a_{j'}^* a_j^* a_{k'})\, a_k - 2\tilde{\omega}(a_{j'}^* a_k a_{k'})\, a_j^* - 2\tilde{\omega}(a_j^* a_k a_{k'})\, a_{j'}^* \Big\} , \end{aligned} \tag{4.74}$$

where $\tilde{\omega}$ is any state, having $(\tilde{\Gamma}, \tilde{v})$ as its admissible pair.

The proof of the following lemma is taken from [8].

**Lemma 4.7 (Fermion Case).** *If the fermionic generalized density matrix $\Gamma$ is a minimizer of (4.66), i. e., if we have $\mathcal{E}_H(\Gamma) = E_{HFB}$, where $\mathcal{E}_H$ is the fermionic energy functional, then $\Gamma$ also fulfills*

$$\mathcal{E}_H^{sc}(\Gamma, \Gamma) = \min \Big\{ \mathcal{E}_H^{sc}(\tilde{\Gamma}, \Gamma) \;\Big|\; \tilde{\Gamma} \text{ admissible generalized density matrix} \Big\} , \tag{4.75}$$

*where $\mathcal{E}_H^{sc}$ is the fermionic self-consistent energy functional.*

*Proof:* Let $\Gamma$ and $\tilde{\Gamma}$ be admissible generalized density matrices. We define a family $\{\Gamma_t\}_{t\in[0,1]}$ of admissible generalized density matrices $\Gamma_t$ by

$$\Gamma_t := (1-t)\cdot\Gamma \;+\; t\cdot\tilde{\Gamma} \quad , \qquad \forall\, t \in [0,1] \,. \tag{4.76}$$

We observe that

$$\Gamma_t = \begin{pmatrix} \gamma_t & \alpha_t \\ -\bar{\alpha}_t & \mathbf{1} - \bar{\gamma}_t \end{pmatrix} \tag{4.77}$$

with

$$\gamma_t = (1-t)\cdot\gamma \;+\; t\cdot\tilde{\gamma} \qquad \text{and} \qquad \alpha_t := (1-t)\cdot\alpha \;+\; t\cdot\tilde{\alpha} \quad , \qquad \forall\, t\in[0,1] \,. \tag{4.78}$$

Recall the definition of $\mathcal{E}_H$ given in (4.67) and note that $\mathcal{E}_H(\Gamma_t)$ is a polynomial of degree two in $t$. It is therefore differentiable and we have

$$\frac{\partial}{\partial t}\mathcal{E}_H(\Gamma_t)\big|_{t=0} = \mathcal{E}_H^{sc}(\tilde{\Gamma}, \Gamma) - \mathcal{E}_H^{sc}(\Gamma, \Gamma) \,. \tag{4.79}$$

To see this, we note that in evaluating the derivative on the left hand side of (4.79) the following terms appear (for convenience, we take the derivatives under the integral sign):

$$\frac{\partial}{\partial t}\operatorname{tr}(h\gamma_t)\big|_{t=0} = \operatorname{tr}(h\tilde{\gamma}) - \operatorname{tr}(h\gamma) \ , \tag{4.80a}$$

$$\begin{aligned}\frac{\partial}{\partial t}\operatorname{tr}(D^2_{r,z}\alpha^*_t D^2_{r,z}\alpha_t)\big|_{t=0} &= \operatorname{tr}\left(D^2_{r,z}(\tilde{\alpha}^* - \alpha^*)D^2_{r,z}\alpha\right) + \operatorname{tr}\left(D^2_{r,z}\alpha^* D^2_{r,z}(\tilde{\alpha} - \alpha)\right) \\ &= 2\operatorname{Re}\operatorname{tr}\left(D^2_{r,z}\tilde{\alpha}^* D^2_{r,z}\alpha\right) - 2\operatorname{tr}\left(D^2_{r,z}\alpha^* D^2_{r,z}\alpha\right) \ ,\end{aligned} \tag{4.80b}$$

$$\begin{aligned}\frac{\partial}{\partial t}\operatorname{tr}\left(D^2_{r,z}\gamma_t D^2_{r,z}\gamma_t\right)\big|_{t=0} &= \operatorname{tr}\left(D^2_{r,z}(\tilde{\gamma} - \gamma)D^2_{r,z}\gamma\right) + \operatorname{tr}\left(D^2_{r,z}\gamma D^2_{r,z}(\tilde{\gamma} - \gamma)\right) \\ &= 2\operatorname{tr}\left(D^2_{r,z}\tilde{\gamma}D^2_{r,z}\gamma\right) + 2\operatorname{tr}\left(D^2_{r,z}\gamma D^2_{r,z}\gamma\right) \ ,\end{aligned} \tag{4.80c}$$

$$\begin{aligned}\frac{\partial}{\partial t}\operatorname{tr}\left(D^2_{r,z}\gamma_t\right)^2\big|_{t=0} &= 2\operatorname{tr}\left(D^2_{r,z}\gamma\right)\operatorname{tr}\left(D^2_{r,z}(\tilde{\gamma} - \gamma)\right) \\ &= 2\operatorname{tr}\left(D^2_{r,z}\tilde{\gamma}\right)\operatorname{tr}\left(D^2_{r,z}\gamma\right) - 2\operatorname{tr}\left(D^2_{r,z}\gamma\right)^2 \ .\end{aligned} \tag{4.80d}$$

Reinserting these expression into (4.67) using (4.70) readily yields (4.79). Suppose $\Gamma$ is a minimizer of (4.66), then the left hand side of (4.79) is larger or equal to 0 for any $\tilde{\Gamma}$. This implies

$$\mathcal{E}^{sc}_H(\tilde{\Gamma}, \Gamma) \geq \mathcal{E}^{sc}_H(\Gamma, \Gamma) \ . \tag{4.81}$$

The lemma is proved. □

We now prove the corresponding lemma in the boson case.

**Lemma 4.8 (Boson Case).** *If the bosonic admissible pair* $(\Gamma, v)$ *is a minimizer of* (4.53), *i. e., if we have* $\mathcal{E}_H\big((\Gamma, v)\big) = E_{HFB}$, *where* $\mathcal{E}_H$ *denotes the bosonic energy functional, then* $(\Gamma, v)$ *also fulfills*

$$\mathcal{E}^{sc}_H\big((\Gamma, v), (\Gamma, v)\big) = \min\left\{ \ \mathcal{E}^{sc}_H\big((\tilde{\Gamma}, \tilde{v}), (\Gamma, v)\big) \ \Big| \ (\tilde{\Gamma}, \tilde{v}) \ \textit{admissible pair} \ \right\} , \tag{4.82}$$

*where* $\mathcal{E}^{sc}_H$ *denotes the bosonic self-consistent energy functional.*

*Proof:* We proceed similarly as in the fermionic case. To any two admissible pairs $(\Gamma, v)$ and $(\tilde{\Gamma}, \tilde{v})$, we assign a family $\{(\Gamma_t, v_t)\}_{t\in[0,1]}$ of admissible pairs by

$$(\Gamma_t, v_t) := \Big((1-t)\cdot\Gamma \ + \ t\cdot\tilde{\Gamma}, \ (1-t)\cdot v \ + \ t\cdot\tilde{v}\Big) \quad , \qquad \forall\, t\in[0,1] \ . \tag{4.83}$$

Recall that the set of admissible pairs is convex by (3.68). Observe that

$$\Gamma_t = \begin{pmatrix} \gamma_t & \alpha_t \\ -\bar{\alpha}_t & -\mathbf{1} - \bar{\gamma}_t \end{pmatrix} , \tag{4.84}$$

with

$$\gamma_t = (1-t)\cdot\gamma \ + \ t\cdot\tilde{\gamma} \qquad \text{and} \qquad \alpha_t = (1-t)\cdot\alpha \ + \ t\cdot\tilde{\alpha} \quad , \qquad \forall\, t\in[0,1] \ . \tag{4.85}$$

Recall the definition of $\mathcal{E}_H$ given in (4.54) and note that $\mathcal{E}_H\big((\Gamma_t, v_t)\big)$ is a polynomial of degree two in $t$. It is therefore differentiable and we have

$$\frac{\partial}{\partial t}\mathcal{E}_H\big((\Gamma_t, v_t)\big)\big|_{t=0} = \mathcal{E}^{sc}_H\big((\tilde{\Gamma}, \tilde{v}), (\Gamma, v)\big) - \mathcal{E}^{sc}_H\big((\Gamma, v), (\Gamma, v)\big) \ . \tag{4.86}$$

To see this, we note that in evaluating the derivative on the left hand side, terms analogous to (4.80) appear. Additionally, we have the following term associated to the one-point functional

$$\begin{aligned}
&\frac{\partial}{\partial t}\left(\sum_{p\in\mathbb{N}} |\,(1-t)\cdot u(D_{r,z}f_p)+t\cdot\tilde{u}(D_{r,z}f_p)\,|^2\right)^2\Bigg|_{t=0} \qquad (4.87)\\
&\quad = 4\sum_{p,q\in\mathbb{N}} \operatorname{Re}\big(\tilde{u}(D_{r,z}f_p)-u(D_{r,z}f_p)\big)\overline{u(D_{r,z}f_p)}\,|\,u(D_{r,z}f_q)\,|^2\\
&\quad = 4\operatorname{Re}\left(\sum_{p\in\mathbb{N}}\tilde{u}(D_{r,z}f_p)\overline{u(D_{r,z}f_p)}\right)\left(\sum_{p\in\mathbb{N}}|\,u(D_{r,z}f_p)\,|^2\right)-4\left(\sum_{p\in\mathbb{N}}|\,u(D_{r,z}f_p)\,|^2\right)^2 .
\end{aligned}$$

Reinserting these expressions into (4.54) using (4.71) readily yields (4.86).

Suppose $(\Gamma, v)$ is a minimizer of (4.53), then the left hand side of (4.86) is larger or equal to zero, for any admissible pair $(\tilde{\Gamma}, \tilde{v})$, implying

$$\mathcal{E}_H^{sc}\big((\tilde{\Gamma},\tilde{v}),(\Gamma,v)\big) \geq \mathcal{E}_H^{sc}\big((\Gamma,v),(\Gamma,v)\big) . \qquad (4.88)$$

The lemma is proved. □

Let us now describe how the above lemmas are used to approximate the HFB-Energy. For simplicity, we consider the fermion case, only. (The boson case is completely analogous.) For a given model, one could now start off with a trial generalized density matrix $\Gamma$ and calculate the minimizer $\tilde{\Gamma}$ of $\mathcal{E}_H^{sc}(\cdot,\Gamma)$. If $\mathcal{E}_H^{sc}(\tilde{\Gamma},\Gamma)$ should turn out be smaller than $\mathcal{E}_H^{sc}(\Gamma,\Gamma)$ one would repeat the same procedure, however starting with $\tilde{\Gamma}$. This procedure is repeated, until eventually equality between $\mathcal{E}_H^{sc}(\tilde{\Gamma},\Gamma)$ and $\mathcal{E}_H^{sc}(\Gamma,\Gamma)$ is achieved. One could then hope, only hope, by the last lemma(s) that $\tilde{\Gamma}$ is in fact the solution to the variational principle (4.66).

# Chapter 5

# Correlation Estimates

## 5.1 Fermionic Theory

### 5.1.1 A Fermionic Wick Theorem

In this subsection we prove a so called Wick Theorem, i. e., a theorem expressing normal-ordered polynomials in the particle creation and annihilation operators in terms of polynomials which are not normal-ordered.

**Definition 5.1.** *Denote by* $a(\cdot)$ *and* $a^*(\cdot)$ *the generators of the CAR Algebra. We then associate to any monomial*

$$a^{\tau_1}(f_1)\cdots a^{\tau_n}(f_n) \quad , \qquad \forall\, n \in \mathbb{N},\ \tau_1,\ldots,\tau_n \in \{\varnothing, *\},\ f_1,\ldots,f_n \in \mathcal{H}^1 \ , \tag{5.1}$$

*a monomial, normal-ordered with respect to the Fock representation, by defining*

$$:a^{\tau_1}(f_1)\cdots a^{\tau_n}(f_n): \ := \ \mathrm{sign}(\pi)\cdot a^{\tau_{\pi(1)}}(f_{\pi(1)})\cdots a^{\tau_{\pi(n)}}(f_{\pi(n)}) \ . \tag{5.2}$$

*The permutation* $\pi$ *is uniquely determined by the conditions*

$$\tau_{\pi(1)} = \cdots = \tau_{\pi(k)} = * \quad , \quad \tau_{\pi(k+1)} = \cdots = \tau_{\pi(n)} = \varnothing \ , \tag{5.3}$$

*for some* $k \in \{0,\ldots,n\}$*, and*

$$\pi(1) < \cdots < \pi(k) \quad , \quad \pi(k+1) < \cdots < \pi(n) \ . \tag{5.4}$$

*By demanding linearity and setting* $:\mathbf{1}: := \mathbf{1}$*, we extend this definition to all polynomials in the fermion annihilation and creation operators and the identity.*

Note that the elements of the CAR Algebra are equivalence classes of polynomials in the generators $a^*(\cdot)$ and $a(\cdot)$. The normal-ordering is defined on these polynomials, but it is *not* well-defined on the CAR Algebra. We discuss these concepts in more detail in Section B.2.

For any homogeneously quadratic, polynomial expression $q$ in the generators of the self-dual CAR Algebra, we define its contraction $[\![q]\!]$ by

$$[\![B(f)B(g)]\!] \ := \ B(f)B(g) - :B(f)B(g): \quad , \qquad \forall\, f,g \in \mathcal{L} \ . \tag{5.5}$$

Note that, for all $f_1, f_2 \in \mathcal{H}^1$ and all $\sigma_1, \sigma_2 \in \{\varnothing, *\}$, the following equality holds:

$$[\![a^{\sigma_1}(f_1)a^{\sigma_2}(f_2)]\!] = \begin{cases} 0 & \text{if } a^{\sigma_1}(f_1)a^{\sigma_2}(f_2) \text{ is normal-ordered} \\ \{a^{\sigma_1}(f_1), a^{\sigma_2}(f_2)\} & \text{else} \end{cases} . \tag{5.6}$$

In order to formulate the fermionic Wick Theorem, we introduce, for any $n \in \mathbb{N}$, the set $\mathcal{P}_2(n)$ as follows: $P$ is an element of $\mathcal{P}_2(n)$ if and only if

$$P = \{ p^{(1)}, \ldots, p^{(k)} \} , \tag{5.7}$$

for some $k \in \mathbb{N}_0$ and some pairwise disjoint sets $p^{(1)}, \ldots, p^{(k)}$ of cardinality two, such that

$$p^{(1)}, \ \ldots, \ p^{(k)} \ \subseteq \ \{1, \ldots, n\} . \tag{5.8}$$

Note that $\varnothing \in \mathcal{P}_2(n)$, for all $n \in \mathbb{N}$ (corresponding to the case $k = 0$). To any $P$ in $\mathcal{P}_2(n)$ we associate a sign, denoted by $\mathrm{sign}(P)$. It is defined to be the sign of any permutation $\pi \in S_n$ satisfying

$$p^{(1)} = \{\pi(1), \pi(2)\} \quad , \quad \ldots \quad , \quad p^{(k)} = \{\pi(2k-1), \pi(2k)\} \tag{5.9}$$

and also satisfying

$$\pi(1) < \pi(2) \ , \ \ldots \ , \ \pi(2k-1) < \pi(2k) \qquad \text{and} \qquad \pi(2k+1) \ < \ \cdots \ < \ \pi(n) \ . \tag{5.10}$$

Note that, even though $\pi$ is not uniquely determined by these conditions, the sign of $\pi$ depends just on $P$, and therefore

$$\mathrm{sign}(P) := \mathrm{sign}(\pi) \tag{5.11}$$

is well-defined.

**Theorem 5.2 (Wick).** *For any $f_1, \ldots, f_n \in \mathcal{H}^1$ and all $\sigma_1, \ldots, \sigma_n \in \{\varnothing, *\}$, let*

$$a_j := a^{\sigma_j}(f_j) \quad , \qquad \forall \ j \in \{1, \ldots, n\} \ . \tag{5.12}$$

*It then holds true that*

$$a_1 \cdots a_n = \sum_{P \in \mathcal{P}_2(n)} \mathrm{sign}(P) \left( \prod_{p \in P} [\![a_{p_1} a_{p_2}]\!] \right) \left( : \prod_{j \in \{1,\ldots,n\} \setminus \bigcup_{p \in P} p} a_j : \right) . \tag{5.13}$$

*The normal-ordered operator product on the right hand side is assumed to be ordered in ascending index order.*

In principle, this theorem can be proved along the same lines as the corresponding Theorem 5.21 in the bosonic context. However, the proof is complicated by the fact that lots of minus signs appear. The best way to deal with this problem is to extend the CAR Algebra by a set of Grassmann variables, as we have indicated in Section C.3. Since in the fermionic context we do not need to generalize the Wick Theorem beyond its well-known form, we omit the proof and refer the reader to [11], see also [6].

An important consequence of relation (5.6) is that any contraction of a monomial of degree two is equal to the vacuum expectation value of this monomial, i. e.,

$$[\![B(f)B(g)]\!] = \Omega\big(B(f)B(g)\big) \quad , \qquad \forall\ f,g \in \mathcal{L}\ . \tag{5.14}$$

It is therefore possible to rewrite the contractions appearing in the Wick Theorem in terms of vacuum expectation values.

For any homogeneous Bogoliubov transformation $w$, denoting by $\alpha_w$ the associated algebra automorphism, we introduce the normal-ordering with respect to $w$ as follows:

$$:\,\cdot\,:_w := \alpha_w^{-1}\big(:\alpha_w\,(\,\cdot\,):\big)\ . \tag{5.15}$$

We generalize the Wick Theorem to the normal-ordering $:\cdot:_w$.

**Corollary 5.3.** *Let $w$ be a fermionic homogeneous Bogoliubov transformation and let $f_1,\dots,f_n \in \mathcal{L}$ be arbitrary. Denote the generators $B(f_1),\dots,B(f_n)$ of the self-dual algebra by $B_1,\dots,B_n$. It then holds*

$$B_1\cdots B_n = \sum_{P\in\mathcal{P}_2(n)} \operatorname{sign}(P)\left(\prod_{p\in P}\Omega_w\left(B_{p_1}B_{p_2}\right)\right)\left(:\prod_{j\in\{1,\dots,n\}\setminus\bigcup_{p\in P}p} B_j:_w\right)\ , \tag{5.16}$$

*where the normal-ordered product on the right hand side is assumed to be in ascending index order and we have denoted*

$$\Omega_w(\cdot) := \Omega\big(\alpha_w(\cdot)\big)\ . \tag{5.17}$$

*Proof:* By additivity, we can apply the Wick Theorem to the generators $\tilde{B}_j := \alpha_w(B_j)$, for all $j \in \{1,\dots,n\}$, to obtain:

$$\begin{aligned}\tilde{B}_1\cdots\tilde{B}_n &= \sum_{P\in\mathcal{P}_2(n)} \operatorname{sign}(P)\left(\prod_{p\in P}[\![\tilde{B}_{p_1}\tilde{B}_{p_2}]\!]\right)\left(:\prod_{j\in\{1,\dots,n\}\setminus\bigcup_{p\in P}p}\tilde{B}_j:\right)\\ &= \sum_{P\in\mathcal{P}_2(n)} \operatorname{sign}(P)\left(\prod_{p\in P}\Omega\left(\tilde{B}_{p_1}\tilde{B}_{p_2}\right)\right)\left(:\prod_{j\in\{1,\dots,n\}\setminus\bigcup_{p\in P}p}\tilde{B}_j:\right)\ ,\end{aligned}$$

where we have used (5.14). From this statement, the claim follows by taking the Bogoliubov transformation $\alpha_w^{-1}$ of both sides and remembering the definition of $\Omega_w$. ☐

We see that in the case $n = 4$, we may rewrite the claim of Corollary 5.3 as follows

$$\begin{aligned}&B_1\cdots B_4 = :B_1\cdots B_4:_w\\ &+\sum_{\pi\ \text{Pairing}}\operatorname{sign}(\pi)\Big\{:B_{\pi(1)}B_{\pi(2)}:_w\,\Omega_w\left(B_{\pi(3)}B_{\pi(4)}\right) + :B_{\pi(3)}B_{\pi(4)}:_w\,\Omega_w\left(B_{\pi(1)}B_{\pi(2)}\right)\Big\}\\ &+\sum_{\pi\ \text{Pairing}}\operatorname{sign}(\pi)\,\Omega_w\left(B_{\pi(1)}B_{\pi(2)}\right)\Omega_w\left(B_{\pi(3)}B_{\pi(4)}\right)\ ,\end{aligned} \tag{5.18}$$

where the sums extend over all pairings, i. e., over all

$$\pi \in S_4 \ , \quad \text{with} \qquad 1 = \pi(1) \ , \quad \pi(2) < \pi(4) \ . \tag{5.19}$$

Observing that

$$:B(f)B(g):_w = B(f)B(g) - \Omega_w\big(B(f)B(g)\big) \quad , \qquad \forall\, f, g \in \mathcal{L} \ , \tag{5.20}$$

we obtain the following corollary.

**Corollary 5.4.** *Under the hypothesis of Corollary 5.3, we have*

$$\begin{aligned} B_1 \cdots B_4 = {} & :B_1 \cdots B_4:_w \\ & + \sum_{\pi \ Pairing} \operatorname{sign}(\pi) \Big\{ B_{\pi(1)} B_{\pi(2)} \Omega_w \left( B_{\pi(3)} B_{\pi(4)} \right) + B_{\pi(3)} B_{\pi(4)} \Omega_w \left( B_{\pi(1)} B_{\pi(2)} \right) \Big\} \\ & - \sum_{\pi \ Pairing} \operatorname{sign}(\pi)\, \Omega_w \left( B_{\pi(1)} B_{\pi(2)} \right) \Omega_w \left( B_{\pi(3)} B_{\pi(4)} \right) \ , \end{aligned}$$

*where the sums extend over all $\pi$ obeying* (5.19)*.*

### 5.1.2 Derivation of the Correlation Estimate

In this subsection we give a lower bound on the expectations of quartic polynomials in the fermion particle annihilation and creation operators of the following type:

$$\sum_{p,q \in \mathbb{N}} :a^*(Df_p) a^*(Df_q) a(Df_q) a(Df_p):_w \ . \tag{5.21}$$

Here, we have fixed an orthonormal basis $\{f_j\}_{j \in \mathbb{N}}$ in $\mathcal{H}^1$ and denoted by $D$ a nonnegative one-particle operator in $\mathcal{B}(\mathcal{H}^1)$. $w$ denotes a homogeneous, up to now unspecified, Bogoliubov transformation. Later, we shall interpret (5.21) as a truncated interaction term.

**Theorem 5.5.** *Suppose we are given an orthonormal basis $\{f_j\}_{j \in \mathbb{N}}$ in $\mathcal{H}^1$, a nonnegative operator $D$ in $\mathcal{B}(\mathcal{H}^1)$ and a homogeneous Bogoliubov transformation $w$ of the form*

$$w = \begin{pmatrix} X & Y \\ \bar{Y} & \bar{X} \end{pmatrix} \ , \qquad \textit{for some} \qquad X, Y \in \mathcal{B}(\mathcal{H}^1) \ , \tag{5.22}$$

*with respect to the decomposition* (1.80)*. We then have the following correlation estimate:*

$$\begin{aligned} & \omega\Bigg( \sum_{p,q \in \mathbb{N}} :a^*(Df_p) a^*(Df_q) a(Df_q) a(Df_p):_w \Bigg) \\ & \geq - 4 \operatorname{tr}\left( D^2 X^* \tilde{\gamma} X \right) \operatorname{tr}\left( \bar{D}^2 Y^* Y \right) \\ & \quad - 4 \operatorname{tr}\left( \bar{D}^2 Y^* Y \right) \sqrt{ \operatorname{tr}\left( \bar{D}^2 Y^* \tilde{\gamma} Y \right) \operatorname{tr}\left( D^2 X^* \tilde{\gamma} X \right) } \\ & \quad - 2 \sqrt{ \operatorname{tr}\left( D^2 X^* \tilde{\gamma} X \right) \operatorname{tr}\left( \bar{D}^2 Y^* Y \right) } \Big[ \operatorname{tr}\left( D^2 Y^T (\mathbf{1} - \bar{\tilde{\gamma}}) \bar{Y} D^2 X^* X \right) \\ & \qquad\qquad + \operatorname{tr}\left( D^2 X^* \tilde{\gamma} X \right) \operatorname{tr}\left( \bar{D}^2 Y^* Y \right) - \operatorname{tr}\left( \bar{D}^2 Y^* X D^2 X^* \tilde{\gamma} Y \right) \\ & \qquad\qquad - \operatorname{tr}\left( \bar{D}^2 Y^* \tilde{\gamma} X D^2 X^* Y \right) + \operatorname{tr}\left( \bar{D}^2 Y^* X D^2 X^* Y \right) \Big]^{\frac{1}{2}} \ , \end{aligned} \tag{5.23}$$

*where $\tilde{\gamma}$ is the transformed reduced density matrix, given by*

$$\tilde{\gamma} := X\gamma_\omega X^* + Y\alpha_\omega^* X + X\alpha_\omega Y^* + Y(\mathbf{1} - \bar{\gamma}_\omega)Y^* \ . \tag{5.24}$$

*Proof:* In order to simplify notation for the purpose of the following, somewhat lengthy calculations, let us abbreviate

$$a_j := a(Df_j) \ , \qquad c_j := a(XDf_j) \ , \qquad d_j := a(Y\overline{Df_j}) \ , \qquad \forall\, j \in \mathbb{N} \ , \tag{5.25}$$

and correspondingly for the adjoints of these operators. On denoting by $\alpha_w$ the algebra automorphism associated to $w$, we observe that

$$\alpha_w(a_r^*) = c_r^* + d_r \quad , \qquad \forall\, r \in \mathbb{N} \ . \tag{5.26}$$

Therefore the expectation of (5.21) in any state $\omega$ is given by

$$\omega\Bigg( \sum_{p,q\in\mathbb{N}} :a_p^* a_q^* a_q a_p:_w \Bigg) = \tilde{\omega}\Bigg( \sum_{p,q\in\mathbb{N}} :(c_p + d_p^*)^*(c_q + d_q^*)^*(c_q + d_q^*)(c_p + d_p^*): \Bigg) \ , \tag{5.27}$$

where we have introduced the transformed state $\tilde{\omega}$, by

$$\tilde{\omega}(\cdot) := \omega\big(\alpha_w^{-1}(\cdot)\big) \ . \tag{5.28}$$

Thus we may write

$$\omega\Bigg( \sum_{p,q\in\mathbb{N}} :a_p^* a_q^* a_q a_p:_w \Bigg) \ = \ \text{expression 1} \ + \ \text{expression 2} \ , \tag{5.29}$$

where

$$\text{expression 1} := \sum_{p,q\in\mathbb{N}} \tilde{\omega}\left( :d_p(c_q + d_q^*)^* d_q^*(c_p + d_p^*): \right) \tag{5.30}$$

and

$$\begin{aligned} \text{expression 2} := \sum_{p,q\in\mathbb{N}} \Big\{ &\tilde{\omega}\left( :d_p(c_q + d_q^*)^* c_q(c_p + d_p^*): \right) \\ &+ \tilde{\omega}\left( :c_p^*(c_q + d_q^*)^* d_q^*(c_p + d_p^*): \right) + \tilde{\omega}\left( :c_p^*(c_q + d_q^*)^* c_q(c_p + d_p^*): \right) \Big\} \ . \end{aligned} \tag{5.31}$$

Note that the normal-ordering applies to the $c$'s and $d$'s appearing in these expressions in just the same way as it does to the $a$'s: Generators bearing a $*$ are moved to the left, keeping track of the minus signs, while suppressing the anti-commutators. We can thus estimate expression 1 in the following way:

$$\begin{aligned} \text{expression 1} &= \sum_{p,q\in\mathbb{N}} \Big\{ \tilde{\omega}(c_q^* d_q^* d_p c_p) - \tilde{\omega}(c_q^* d_q^* d_p^* d_p) + \tilde{\omega}(d_q^* d_p d_q c_p) + \tilde{\omega}(d_q^* d_p^* d_p d_q) \Big\} \\ &\geq -2 \sum_{p,q\in\mathbb{N}} \big| \tilde{\omega}(d_q^* d_p d_q c_p) \big| \geq -2 \left[ \sum_{p,q\in\mathbb{N}} \tilde{\omega}(d_q^* d_p d_p^* d_q) \right]^{\frac{1}{2}} \left[ \sum_{p,q\in\mathbb{N}} \tilde{\omega}(c_p^* d_q^* d_q c_p) \right]^{\frac{1}{2}} \\ &\geq -2 \left[ \sum_{p,q\in\mathbb{N}} \{d_p^*, d_p\}\, \tilde{\omega}(d_q^* d_q) \right]^{\frac{1}{2}} \left[ \sum_{p,q\in\mathbb{N}} \{d_q^*, d_q\}\, \tilde{\omega}(c_p^* c_p) \right]^{\frac{1}{2}} \ . \end{aligned} \tag{5.32}$$

In the first step of this estimate, we drop the first and the last expectation value, since they are obviously positive (note that the remaining two term are conjugate to each other, after performing an anti-commutation in one of them). We then use the Cauchy-Schwarz estimate first on $\tilde{\omega}$ and again on the sum over $p$ and $q$. Finally, we estimate according to

$$AA^* = \{A, A^*\} - A^*A \leq \{A, A^*\} \quad , \qquad \forall\ A \in \mathcal{B}(\mathcal{H}^1) \tag{5.33}$$

Note that

$$\begin{aligned} \text{expression 2} = \sum_{p,q\in\mathbb{N}} \Big\{ & \tilde{\omega}\big(:d_p c_q^* c_q c_p:\big) + \tilde{\omega}\big(:d_p c_q^* c_q d_p^*:\big) + \tilde{\omega}\big(:d_p d_q c_q c_p:\big) \\ & + \tilde{\omega}\big(:d_p d_q c_q d_p^*:\big) + \tilde{\omega}\big(:c_p^* c_q^* d_q^* c_p:\big) + \tilde{\omega}\big(:c_p^* c_q^* d_q^* d_p^*:\big) \\ & + \tilde{\omega}\big(:c_p^* d_q d_q^* c_p:\big) + \tilde{\omega}\big(:c_p^* d_q d_q^* d_p^*:\big) + \tilde{\omega}\big(:c_p^* c_q^* c_q c_p:\big) \\ & + \tilde{\omega}\big(:c_p^* c_q^* c_q d_p^*:\big) + \tilde{\omega}\big(:c_p^* d_q c_q c_p:\big) + \tilde{\omega}\big(:c_p^* d_q c_q d_p^*:\big) \Big\} \ . \end{aligned} \tag{5.34}$$

We further subdivide expression 2 into four groups of subexpressions, as follows.

$$\text{expression 2} \ = \ \text{group 1} \ + \ \text{group 2} \ + \ \text{group 3} \ + \ \text{group 4}\ , \tag{5.35}$$

with

$$\begin{aligned} \text{group 1} := \sum_{p,q\in\mathbb{N}} \Big\{ & -\tilde{\omega}(c_q^* d_p c_q c_p) - \tilde{\omega}(c_q^* d_p^* d_p c_q) + \tilde{\omega}(c_p^* c_q^* d_q^* c_p) - \tilde{\omega}(c_p^* d_q^* d_q c_p) \\ & + \tilde{\omega}(c_p^* c_q^* c_q c_p) - \tilde{\omega}(c_p^* c_q^* d_p^* c_q) + \tilde{\omega}(c_p^* d_q c_q c_p) \Big\} \ , \end{aligned} \tag{5.36}$$

$$\text{group 2} := \sum_{p,q\in\mathbb{N}} \Big\{ -\tilde{\omega}(d_p^* d_p d_q c_q) + \tilde{\omega}(c_p^* d_q^* d_p^* d_q) \Big\} \ , \tag{5.37}$$

$$\text{group 3} := \sum_{p,q\in\mathbb{N}} \Big\{ \tilde{\omega}(d_p d_q c_q c_p) + \tilde{\omega}(c_p^* c_q^* d_q^* d_p^*) \Big\} \ , \tag{5.38}$$

$$\text{group 4} := \sum_{p,q\in\mathbb{N}} \tilde{\omega}(c_p^* d_p^* d_q c_q) \ . \tag{5.39}$$

We estimate these groups of expressions.

$$\begin{aligned} \text{group 1} &= \sum_{p,q\in\mathbb{N}} \Big\{ \tilde{\omega}(c_p^* c_q^* c_q c_p) + 4\,\mathrm{Re}\,\tilde{\omega}(c_p^* d_q c_q c_p) - 2\tilde{\omega}(c_q^* d_p^* d_p c_q) \Big\} \\ &\geq \sum_{p,q\in\mathbb{N}} \Big\{ \tilde{\omega}(c_p^* c_q^* c_q c_p) - 4\sqrt{\tilde{\omega}(c_p^* d_q d_q^* c_p)}\sqrt{\tilde{\omega}(c_p^* c_q^* c_q c_p)} - 2\tilde{\omega}(c_q^* d_p^* d_p c_q) \Big\} \\ &\geq \sum_{p,q\in\mathbb{N}} \big\{ -4\tilde{\omega}(c_p^* d_q d_q^* c_p) - 2\tilde{\omega}(c_q^* d_p^* d_p c_q) \big\} \geq -4 \sum_{p,q\in\mathbb{N}} \tilde{\omega}(c_p^* c_p) \left\{ d_q, d_q^* \right\} \ . \end{aligned} \tag{5.40}$$

Here, in a first step, we use the Cauchy-Schwarz estimate on $\tilde{\omega}$ in the middle term. Then we complete a square, thus generating a positive term, which we drop. On the left hand side of the last line, the terms partially cancel each other. Finally, we use (5.33), again.

$$\begin{aligned} \text{group 2} = 2 \sum_{p,q\in\mathbb{N}} \mathrm{Re}\ \tilde{\omega}(d_p^* d_q d_p c_q) &\geq -2 \sqrt{\sum_{p,q\in\mathbb{N}} \tilde{\omega}(d_p^* d_q d_q^* d_p)} \sqrt{\sum_{p,q\in\mathbb{N}} \tilde{\omega}(c_q^* d_p^* d_p c_q)} \\ &\geq -2 \sqrt{\sum_{p,q\in\mathbb{N}} \tilde{\omega}(d_p^* d_p) \left\{ d_q, d_q^* \right\}} \sqrt{\sum_{p,q\in\mathbb{N}} \tilde{\omega}(c_q^* c_q) \left\{ d_p, d_p^* \right\}} \ . \end{aligned} \tag{5.41}$$

Here, we use the Cauchy-Schwarz estimate first on the state $\tilde{\omega}$ and afterwards on the summation over $p$ and $q$. After that, we use estimate (5.33) on each of the resulting factors.

$$\begin{aligned}
&\text{group } 3 = 2 \sum_{p,q\in\mathbb{N}} \operatorname{Re}\, \tilde{\omega}(c_q^* d_q^* c_p^* d_p^*) \\
&= -2\tilde{\omega}\left(\Big(\sum_{q\in\mathbb{N}} c_q^* d_q^*\Big)\Big(\sum_{p\in\mathbb{N}} c_p^* d_p^*\Big)\right) \geq -2 \underbrace{\sqrt{\sum_{p,q\in\mathbb{N}} \tilde{\omega}(c_q^* d_q^* d_p c_p)}}_{\text{factor 1}}\ \underbrace{\sqrt{\sum_{p,q\in\mathbb{N}} \tilde{\omega}(d_q c_q c_p^* d_p^*)}}_{\text{factor 2}}\ . \qquad (5.42)
\end{aligned}$$

For a change, we use here the Cauchy-Schwarz estimate on the state $\tilde{\omega}$. We now estimate the two factors on the right hand side separately.

$$\text{factor 1} \leq \sum_{q\in\mathbb{N}} \sqrt{\tilde{\omega}(c_q^* d_q^* d_q c_q)} \leq \sqrt{\sum_{p,q\in\mathbb{N}} \tilde{\omega}(c_q^* c_q)\left\{d_p^*, d_p\right\}}\ , \qquad (5.43)$$

$$\text{factor 2} \leq \sqrt{\sum_{p,q\in\mathbb{N}} \tilde{\omega}(d_q d_p^*)\left\{c_q, c_p^*\right\} + \sum_{p,q\in\mathbb{N}} \left|\,\tilde{\omega}(d_q c_p^* c_q d_p^*)\,\right|}\ . \qquad (5.44)$$

The second sum under the square root in factor 2 is in turn estimated as follows:

$$\begin{aligned}
\sum_{p,q\in\mathbb{N}} \left|\,\tilde{\omega}(d_q c_p^* c_q d_p^*)\,\right| &\leq \sum_{p,q\in\mathbb{N}} \sqrt{\tilde{\omega}(d_q c_p^* c_p d_q^*)}\sqrt{\tilde{\omega}(d_p c_q^* c_q d_p^*)} \\
&\leq \sqrt{\sum_{p,q\in\mathbb{N}} \tilde{\omega}(d_q c_p^* c_p d_q^*)}\sqrt{\sum_{p,q\in\mathbb{N}} \tilde{\omega}(d_p c_q^* c_q d_p^*)} \\
&= \sum_{p,q\in\mathbb{N}} \tilde{\omega}(d_p c_q^* c_q d_p^*) \\
&= \sum_{p,q\in\mathbb{N}} \tilde{\omega}\Big(\big[c_q^* d_p - \left\{c_q^*, d_p\right\}\big]\ \big[d_p^* c_q - \left\{d_p^*, c_q\right\}\big]\Big) \\
&\leq \sum_{p,q\in\mathbb{N}} \Big[\tilde{\omega}(c_q^* c_q)\left\{d_p, d_p^*\right\} - \tilde{\omega}(d_p^* c_q)\left\{c_q^*, d_p\right\} \\
&\qquad - \tilde{\omega}(c_q^* d_p)\left\{d_p^*, c_q\right\} + \left\{d_p^*, c_q\right\}\left\{c_q^*, d_p\right\}\Big]\ . \qquad (5.45)
\end{aligned}$$

Here, we use the Cauchy-Schwarz estimate two times, once on $\tilde{\omega}$ and then on the sum over $p$ and $q$, thus simplifying the indices. Then, we commute the $c$'s with the $d$'s and finally use (5.33) on the only remaining quartic term. Thus we obtain the following estimate on group 3:

$$\begin{aligned}
&\text{group } 3 \geq -2 \sqrt{\sum_{p,q\in\mathbb{N}} \tilde{\omega}(c_q^* c_q)\left\{d_p^*, d_p\right\}}\ \Bigg[\sum_{p,q\in\mathbb{N}} \Big(\left\{d_q^*, d_p\right\} - \tilde{\omega}(d_q^* d_p)\Big)\left\{c_q^*, c_p\right\} \\
&+ \sum_{p,q\in\mathbb{N}} \Big(\tilde{\omega}(c_q^* c_q)\left\{d_p, d_p^*\right\} - \tilde{\omega}(d_p^* c_q)\left\{c_q^*, d_p\right\} - \tilde{\omega}(c_q^* d_p)\left\{d_p^*, c_q\right\} + \left\{d_p^*, c_q\right\}\left\{c_q^*, d_p\right\}\Big)\Bigg]^{\frac{1}{2}}\ . \qquad (5.46)
\end{aligned}$$

From the terms in expression 2 only one term remains:

$$\text{group } 4 = \sum_{p,q\in\mathbb{N}} \tilde{\omega}(c_p^* d_p^* d_q c_q) \geq 0 \ . \tag{5.47}$$

We have now estimated all the sixteen terms resulting from the right hand side of (5.27). The remaining expectation values and anti-commutators have the following explicit forms:

$$\begin{aligned}
\{c_j^*, c_{j'}\} &= \langle f_{j'} \,|\, DX^*XDf_j \rangle \ , & \tilde{\omega}(c_j^* c_{j'}) &= \langle f_{j'} \,|\, DX^*\tilde{\gamma}XDf_j \rangle \ , \\
\{c_j^*, d_{j'}\} &= \langle \bar{f}_{j'} \,|\, \bar{D}Y^*XDf_j \rangle \ , & \tilde{\omega}(c_j^* d_{j'}) &= \langle \bar{f}_{j'} \,|\, \bar{D}Y^*\tilde{\gamma}XDf_j \rangle \ , \\
\{d_j^*, c_{j'}\} &= \langle f_{j'} \,|\, DX^*Y\bar{D}\bar{f}_j \rangle \ , & \tilde{\omega}(d_j^* c_{j'}) &= \langle f_{j'} \,|\, DX^*\tilde{\gamma}Y\bar{D}\bar{f}_j \rangle \ , \\
\{d_j^*, d_{j'}\} &= \langle \bar{f}_{j'} \,|\, \bar{D}Y^*Y\bar{D}\bar{f}_j \rangle \ , & \tilde{\omega}(d_j^* d_{j'}) &= \langle \bar{f}_{j'} \,|\, \bar{D}Y^*\tilde{\gamma}Y\bar{D}\bar{f}_j \rangle \ .
\end{aligned}$$

Here, we have denoted by $\tilde{\gamma}$ the density matrix of the state $\tilde{\omega}$, the connection being given by

$$\langle f \,|\, \tilde{\gamma} g \rangle = \tilde{\omega}\big(a^*(g)a(f)\big) \quad , \qquad \forall\ f,g \in \mathcal{H}^1 \ . \tag{5.48}$$

We remark that

$$\begin{aligned}
\langle f \,|\, \tilde{\gamma} g \rangle &= \omega\Big(\big(a^*(X^*g) + a(Y^T\bar{g})\big)\big(a(X^*f) + a^*(Y^T\bar{f})\big)\Big) \\
&= \big\langle f \,\big|\, \big(X\gamma_\omega X^* + Y\alpha_\omega^* X^* + X\alpha_\omega Y^* + Y(\mathbf{1} - \bar{\gamma}_\omega)Y^*\big)g \big\rangle \ ,
\end{aligned} \tag{5.49}$$

see (5.24). Inserting these explicit forms into expression 1, we obtain

$$\text{expression } 1 \geq -2\,\mathrm{tr}\left(\bar{D}Y^*Y\right) \sqrt{\mathrm{tr}\left(\bar{D}^2Y^*\tilde{\gamma}Y\right) \mathrm{tr}\left(D^2X^*\gamma X\right)} \ . \tag{5.50}$$

Inserting these explicit forms into the estimates of groups 1-3, we obtain

$$\text{group } 1 \geq -4\,\mathrm{tr}\left(D^2X^*\tilde{\gamma}X\right) \mathrm{tr}\left(\bar{D}^2Y^*Y\right) \ , \tag{5.51}$$

$$\text{group } 2 \geq -2\,\mathrm{tr}\left(\bar{D}^2Y^*Y\right) \sqrt{\mathrm{tr}\left(\bar{D}^2Y^*\tilde{\gamma}Y\right) \mathrm{tr}\left(D^2X^*\tilde{\gamma}X\right)} \ , \tag{5.52}$$

$$\begin{aligned}
\text{group } 3 \geq 2\sqrt{\mathrm{tr}\left(D^2X^*\tilde{\gamma}X\right) \mathrm{tr}\left(\bar{D}^2Y^*Y\right)} \Big[ &\mathrm{tr}\left(D^2Y^T(1-\bar{\tilde{\gamma}})\bar{Y}D^2X^*X\right) \\
&+ \mathrm{tr}\left(D^2X^*\tilde{\gamma}X\right) \mathrm{tr}\left(\bar{D}^2Y^*Y\right) - \mathrm{tr}\left(\bar{D}^2Y^*XD^2X^*\tilde{\gamma}Y\right) \\
&- \mathrm{tr}\left(\bar{D}^2Y^*\tilde{\gamma}XD^2X^*Y\right) + \mathrm{tr}\left(\bar{D}^2Y^*XD^2X^*Y\right) \Big]^{\frac{1}{2}} \ .
\end{aligned} \tag{5.53}$$

Collecting estimates (5.51)-(5.53) and (5.47) yields an estimate for expression 2 by (5.35). This together with (5.50) is the right hand side of the inequality in the claim of the theorem. □

### 5.1.3 The Role of the Correlation Estimate

We now bring together the results of the preceeding sections of the present chapter with the ideas of HFB-Theory formulated in Chapter 4. The aim is to use the correlation estimate to control the error resulting from approximating the ground state energy by $E_{HFB}$. In particular, we give a lower bound on $E_0$.

First, we note that the energy expectation $\omega(H)$ is not yet defined for a general admissible state $\omega$, possibly not quasi-free. If we knew that the two-particle density matrix $M_\omega$ was a trace-class operator in $\mathcal{H}^2$, we could make sense of this quantity by (4.61) ($\gamma_\omega$ is trace-class by admissibility). However, since we are "only" interested in a lower bound on $\omega(H)$, it suffices to consider states $\omega$ with precisely this property. (Note that $M_\omega$ is in any case nonnegative.) This assertion remains to be proved.

In order to make contact between the ideas presented in this chapter and those presented in the previous one, we first note that

$$\begin{aligned}\operatorname{tr}\left(D_{r,z}^2 \otimes D_{r,z}^2\, M_\omega\right) &= \sum_{p,q\in\mathbb{N}} \left\langle (D_{r,z} f_q) \otimes (D_{r,z} f_p) \;\middle|\; M_\omega\, (D_{r,z} f_q) \otimes (D_{r,z} f_p) \right\rangle \\ &= \sum_{p,q\in\mathbb{N}} \omega\big(a^*(D_{r,z} f_p) a^*(D_{r,z} f_q) a(D_{r,z} f_q) a(D_{r,z} f_p)\big) \ . \end{aligned} \tag{5.54}$$

We can now use Corollary 5.4 to expand the quartic expectation value, given an arbitrary homogeneous Bogoliubov transformation $w$, to obtain:

$$\begin{aligned}\operatorname{tr}\left(D_{r,z}^2 \otimes D_{r,z}^2\, M_\omega\right) &= \mathcal{W}_{r,z}(\Gamma_\omega, \Gamma_{\Omega_w}) - \frac{1}{2}\mathcal{W}_{r,z}(\Gamma_{\Omega_w}, \Gamma_{\Omega_w}) \\ &\quad + \sum_{p,q\in\mathbb{N}} \omega\big({:}\, a^*(D_{r,z} f_p) a^*(D_{r,z} f_q) a(D_{r,z} f_q) a(D_{r,z} f_p) \,{:}_w\big) \ . \end{aligned} \tag{5.55}$$

Here, we have denoted $\Omega_w(\cdot) := \Omega\big(\alpha_w(\cdot)\big)$ and defined the self-consistent interaction term

$$\mathcal{W}_{r,z}(\Gamma, \tilde\Gamma) := 2\operatorname{Re}\operatorname{tr}\left(D_{r,z}^2 \alpha^* D_{r,z}^2 \tilde\alpha\right) - 2\operatorname{tr}\left(D_{r,z}^2 \gamma D_{r,z}^2 \tilde\gamma\right) + 2\operatorname{tr}\left(D_{r,z}^2 \gamma\right)\operatorname{tr}\left(D_{r,z}^2 \tilde\gamma\right) \ , \tag{5.56}$$

for any two admissible generalized density matrices

$$\Gamma = \begin{pmatrix} \gamma & \alpha \\ -\bar\alpha & \mathbf{1} - \bar\gamma \end{pmatrix} \qquad \text{and} \qquad \tilde\Gamma = \begin{pmatrix} \tilde\gamma & \tilde\alpha \\ -\bar{\tilde\alpha} & \mathbf{1} - \bar{\tilde\gamma} \end{pmatrix} \ . \tag{5.57}$$

Note that the self-consistent interaction term $\mathcal{W}_{r,z}(\Gamma, \tilde\Gamma)$ coincides with the interaction term of the fermionic self-consistent energy functional $\mathcal{E}_H^{sc}(\Gamma, \tilde\Gamma)$. Thus the correlation estimates controls, up to the offset term $\frac{1}{2}\mathcal{W}_{r,z}(\Gamma_{\Omega_w}, \Gamma_{\Omega_w})$, the error resulting from replacing the true energy expectation value by the self-consistent energy functional for the trial state given by $\Omega_w$.

### 5.1.4 Application to the Fermionic Jellium Model

In this subsection, we bring to bear the tools developed in the previous sections and chapters to the Fermionic Jellium Model. In a slightly different form, involving different boundary conditions, this problem was already discussed by Graf and Solovej in [19].

#### Description of the Model

We consider a many-fermion system over the one-particle space $\mathcal{H}^1$ given by

$$\mathcal{H}^1 = L^2(\Lambda) \qquad \text{and} \qquad \Lambda := (\mathbb{R}/L\mathbb{Z})^3 \ , \tag{5.58}$$

for any size parameter $L > 0$. Furthermore, we define the conjugation mapping

$$\overline{(\,\cdot\,)} : L^2(\Lambda) \to L^2(\Lambda) \;, \qquad \bar{\psi}(x) := \overline{\psi(x)} \quad , \qquad \forall\, x \in \Lambda \;. \tag{5.59}$$

For any operator $A \in \mathcal{B}(\mathcal{H}^1)$, we define the conjugate operator $\bar{A} \in \mathcal{B}(\mathcal{H}^1)$ by

$$\bar{A}\psi \;:=\; \overline{A\bar{\psi}} \quad , \qquad \forall\, \psi \in \mathcal{H}^1 \;. \tag{5.60}$$

Let the interaction term, as described in (4.6), be given by a pair-potential $v$ allowing a decomposition as discussed in Section 4.1, i. e.,

$$v(x-y) = \int_0^\infty dr\, g(r) \int_\Lambda d^3z\, d_r(x-z)\, d_r(y-z) \quad , \qquad \forall\, x, y \in \Lambda,\; x \neq y \;, \tag{5.61}$$

for a measurable, nonnegative weight function $g$ on $\mathbb{R}^+$ and a family $\{d_r\}_{r>0}$ of bounded, nonnegative and measurable localization functions $d_r$ on $\Lambda$.

The following arguments will be formulated for any such pair-potential. Whenever we need to make some assumptions on the localization functions $\{d_r\}_{r>0}$ and/or the weight function $g$, we resort to the test-case scenario given by the Yukawa Potential $v_\nu$ on the torus, defined for $\nu \geq 0$ in (4.34). In the course of the our calculations, we will introduce several constants, depending on the exact choice for $v$. All these constants are finite, for $v = v_\nu$ and any $\nu > 0$. Some of these constants are, however, not uniformly bounded as $\nu \to 0^+$. We recall that we define the bounded, nonnegative operators $D_{r,z}$ on $\mathcal{H}^1$ by

$$D_{r,z}\psi(x) := d_r(x-z)^{\frac{1}{2}}\psi(x) \quad , \qquad \forall\, x \in \Lambda,\; r > 0,\; z \in \Lambda \;. \tag{5.62}$$

Let the one-particle Hamiltonian $h$ in (4.5) be given by

$$h_\varrho := -\triangle - J_\varrho \cdot \mathbf{1} \;, \tag{5.63}$$

for any density parameter $\varrho > 0$. The number $J_\varrho$ is defined by

$$J_\varrho := \varrho\lambda \int_\Lambda d^3x\, v(x) \;. \tag{5.64}$$

$\lambda > 0$ plays the role of a coupling parameter. Note that $J_\varrho$ is finite in the case $v = v_\nu$, for all $\nu > 0$. The Laplace operator $\triangle$ on the torus $\Lambda$ is defined on the domain

$$\mathcal{D}(\triangle) := \left\{ f \in \mathcal{H}^1 \;\Big|\; \sum_{k \in \Lambda^*} k^2 \left| \hat{f}_k \right|^2 < \infty \right\} , \tag{5.65}$$

where we have denoted

$$\Lambda^* := \left( \frac{2\pi}{L}\mathbb{Z} \right)^3 \tag{5.66}$$

and

$$\hat{f}_k := \langle \phi_k \,|\, f \rangle \;, \qquad \text{with} \qquad \phi_k(x) := \frac{e^{ik\cdot x}}{L^{\frac{3}{2}}} \quad , \qquad \forall\, k \in \Lambda^*,\; x \in \Lambda \;. \tag{5.67}$$

The numbers $\hat{f} := \{\hat{f}_k\}_{k\in\Lambda^*}$ are of course the Fourier coefficients of $f$. Note that $\{\phi_k\}_{k\in\Lambda^*}$ is an orthonormal basis in $\mathcal{H}^1$, and therefore the mapping $f \mapsto \hat{f}$ is unitary, if $\hat{f}$ is considered as an element of $\ell^2(\Lambda^*)$. We simply define

$$(-\triangle)f \ := \ \sum_{k\in\Lambda^*} \left(k^2 \hat{f}_k\right)\phi_k \quad , \qquad \forall\ f \in \mathcal{D}(\triangle)\ . \tag{5.68}$$

In the sequel of this subsection we shall be interested in the expectation values of the Hamilton operator $H_\varrho$ associated to the one-particle operator $h_\varrho$ and the pair-potential $\lambda \cdot v$. Even though the definition of $H_\varrho$ in (4.5) is just formal, we have specified how we make sense of the expectation values of $H_\varrho$ in an admissible state $\omega$. Namely, we have

$$\omega\left(H_\varrho\right) := \mathrm{tr}\left((h_\varrho - \mu\cdot\mathbf{1})\gamma_\omega\right) + \frac{\lambda}{2}\int_0^\infty dr\, g(r)\int_\Lambda d^3z\ \mathrm{tr}\left(D_{r,z}^2 \otimes D_{r,z}^2\, M_\omega\right)\ . \tag{5.69}$$

$M_\omega$ denotes the two-particle density matrix of $\omega$. Additionally to the assumption that $\omega$ is admissible, we also assume that $M_\omega$ is trace-class. The parameter $\mu > 0$ plays the role of a chemical potential. For any given $\varrho > 0$, we adjust it to the value

$$\mu = \left(6\pi^2\varrho\right)^{\frac{2}{3}}\ . \tag{5.70}$$

### Introducing the Variational Principle

We now use (5.55) to rewrite the energy expectation (5.69), where we choose the following homogenous Bogoliubov transformation $w_\mu$:

$$w_\mu = \begin{pmatrix} P_\mu^\perp & P_\mu \\ P_\mu & P_\mu^\perp \end{pmatrix}\ , \quad \text{with} \qquad P_\mu = \bar{P}_\mu := \chi_{[0,\mu]}(-\triangle)\ . \tag{5.71}$$

The fact that $\bar{P}_\mu = P_\mu$ (and $\bar{P}_\mu^\perp = P_\mu^\perp$) follows easily from the definition of $-\triangle$, see (5.68), and the definition of the conjugation, see (5.60). It is easy to see that $w_\mu$ is indeed unitary in $\mathcal{L}$ and fulfills $\tau w_\mu \tau = w_\mu$. It is, hence, a homogenous Bogoliubov transformation. We may therefore rewrite $\omega\left(H_\varrho\right)$ by (5.55) according to

$$\begin{aligned}\omega\left(H_\varrho\right) = \mathrm{tr}\left((h_\varrho - \mu)\gamma\right) + \frac{\lambda}{2}\int_0^\infty dr\, g(r)\int_\Lambda d^3z \Big\{ &\mathcal{W}_{r,z}(\Gamma_\omega, \Gamma_\mu) - \frac{1}{2}\mathcal{W}_{r,z}(\Gamma_\mu, \Gamma_\mu) \\ &+ \sum_{p,q\in\mathbb{N}} \omega\big(:a^*(D_{r,z}f_p)a^*(D_{r,z}f_q)a(D_{r,z}f_q)a(D_{r,z}f_p):_\mu\big)\Big\}\ ,\end{aligned} \tag{5.72}$$

where we have abbreviated:

$$:\cdots:_\mu \ := \ :\cdots:_{w_\mu} \qquad \text{and} \qquad \Gamma_\mu \ := \ \Gamma_{\Omega_\mu}\ . \tag{5.73}$$

We denoted

$$\Omega_\mu(\cdot) := \Omega\big(\alpha_{w_\mu}(\cdot)\big)\ . \tag{5.74}$$

Recall the definition of the self-consistent interaction term $\mathcal{W}_{r,z}$ given in (5.56). Furthermore, we note that the off-diagonal entries of $\Gamma_\mu$ actually vanish. More precisely, we have

$$\Gamma_\mu = \begin{pmatrix} P_\mu & \mathbf{0} \\ \mathbf{0} & P_\mu^\perp \end{pmatrix}\ . \tag{5.75}$$

This entails the following simplification compared to (5.56):

$$\mathcal{W}_{r,z}(\Gamma_\omega, \Gamma_\mu) = -\underbrace{2\,\mathrm{tr}\left(D^2_{r,z}\gamma_\omega D^2_{r,z}P_\mu\right)}_{\text{indirect part}} + \underbrace{2\,\mathrm{tr}\left(D^2_{r,z}\gamma_\omega\right)\mathrm{tr}\left(D^2_{r,z}P_\mu\right)}_{\text{direct part}} , \tag{5.76}$$

$$\mathcal{W}_{r,z}(\Gamma_\mu, \Gamma_\mu) = -\underbrace{2\,\mathrm{tr}\left(D^2_{r,z}P_\mu D^2_{r,z}P_\mu\right)}_{\text{indirect part}} + \underbrace{2\,\mathrm{tr}\left(D^2_{r,z}P_\mu\right)^2}_{\text{direct part}} . \tag{5.77}$$

Before we begin with estimating the right hand side of (5.72), we simplify the problem as follows.

**Lemma 5.6.** *For any admissible, fermionic state $\omega$ such that its two-particle density matrix is trace-class, we have, for any chemical potential $\mu > 0$, any coupling $\lambda > 0$ and any density $\varrho > 0$,*

$$\begin{aligned}
\omega\left(H_\varrho\right) = &\ \mathrm{tr}\left((-\triangle - \mu \cdot \mathbf{1})\gamma_\omega\right) \\
&- \lambda \int_0^\infty dr\, g(r) \int_\Lambda d^3z\ \mathrm{tr}\left(D^2_{r,z}(\gamma_\omega - P_\mu)D^2_{r,z}P_\mu\right) \\
&- \frac{\lambda}{2}\int_0^\infty dr\, g(r) \int_\Lambda d^3z\ \mathrm{tr}\left(D^2_{r,z}P_\mu D^2_{r,z}P_\mu\right) - \frac{\lambda}{2}L^3 g_6 b_1^2 \varrho^2 \\
&+ \frac{\lambda}{2}\int_0^\infty dr\, g(r) \int_\Lambda d^3z \sum_{p,q\in\mathbb{N}} \omega\big(:a^*(D_{r,z}f_p)a^*(D_{r,z}f_q)a(D_{r,z}f_q)a(D_{r,z}f_p):_\mu\big) \\
&+ O(L^2) + O(L^{-1})\,\mathrm{tr}\left(\gamma_\omega\right) ,
\end{aligned} \tag{5.78}$$

*where*

$$g_s := \int_0^\infty dr\, g(r) r^s \qquad \text{and} \qquad b_n := \int_\Lambda d^3x\, d_1(x)^n , \tag{5.79}$$

*for all $n \in \mathbb{N}$ and all $s \geq 0$. Moreover, $g_6$ and $b_1$ are finite if $v = v_\nu$, for some $\nu > 0$.*

Before we go into the proof of the lemma (see p. 107), let us single out the following subexpressions on the right hand side of (5.78) for future reference:

$$T_\mu(\gamma) := \mathrm{tr}\left((-\triangle - \mu\cdot\mathbf{1})\gamma\right) , \tag{5.80}$$

$$I^{(1)}_\mu(\gamma) := \int_0^\infty dr\, g(r)\int_\Lambda d^3z\ \mathrm{tr}\left(D^2_{r,z}(\gamma - P_\mu)D^2_{r,z}P_\mu\right) , \tag{5.81}$$

$$I^{(2)}_\mu := \int_0^\infty dr\, g(r)\int_\Lambda d^3z\ \mathrm{tr}\left(D^2_{r,z}P_\mu D^2_{r,z}P_\mu\right) , \tag{5.82}$$

$$Z_\mu(\omega) := \int_0^\infty dr\, g(r)\int_\Lambda d^3z \sum_{p,q\in\mathbb{N}} \omega\big(:a^*(D_{r,z}f_p)a^*(D_{r,z}f_q)a(D_{r,z}f_q)a(D_{r,z}f_p):_\mu\big) , \tag{5.83}$$

for any $\mu \geq 0$ and any admissible state $\omega$ and any trace-class density matrix $\gamma$.

**Remark 5.7:** Let $f : \mathbb{R}^+_0 \to \mathbb{R}$ be a function. We then write

$$f(L) = O(L^\alpha) , \tag{5.84}$$

for any real $\alpha$, if and only if

$$\left|\frac{f(L)}{L^\alpha}\right| < c \quad , \qquad \forall\ L > L_0 , \tag{5.85}$$

for some $L_0 > 0$ and some $c > 0$. To be precise, we note that $O(L^\alpha)$ is not itself a function. It is rather an equivalence class of functions and the significance of (5.84) is that $f$ is an element of this class.

Numerical factors and factors not dependent on $L$, such as $\lambda$ and $\varrho$, may therefore be absorbed into the $O(L^\alpha)$ terms. For example, we may write

$$2\lambda\varrho O(L^\alpha) = O(L^\alpha) \ . \tag{5.86}$$

Equality is understood as the equality of equivalence classes. Factors depending on the state $\omega$, however, may not be absorbed, since $\omega$ may depend on $L$. (This is because we are looking for a state $\omega$ with minimal energy.)

*Proof of Lemma 5.6:* The starting point of the proof are (5.72), (5.76) and (5.77). First, we calculate the direct parts in (5.76) and (5.77). By expanding the trace in the orthonormal basis $\{\phi_k\}_{k\in\Lambda^*}$ given in (5.67), we have

$$\operatorname{tr}\left(D_{r,z}^{2n} P_\mu\right) = \sum_{k\in\Lambda_\mu^*} \left\langle \phi_k \,\middle|\, D_{r,z}^{2n}\phi_k \right\rangle = \frac{1}{L^3}\sum_{k\in\Lambda_\mu^*} \int_\Lambda d^3x\, d_r^n(x-z) = \frac{|\,\Lambda_\mu^*\,|}{L^3} r^3 b_n \ , \tag{5.87}$$

for all $n\in\mathbb{N}$, with

$$\Lambda_\mu^* := \left\{ k\in\Lambda^* \;\middle|\; |\,k\,|^2 \le \mu \right\} \ . \tag{5.88}$$

We observe that asymptotically, for large $L$, the number of elements of $\Lambda_\mu^*$ is given by

$$\operatorname{tr}(P_\mu) = |\,\Lambda_\mu^*\,| = \varrho L^3 + O\left(L^2\right) \ . \tag{5.89}$$

Thus we obtain for the direct part in (5.77):

$$\operatorname{tr}\left(D_{r,z}^{2n} P_\mu\right) = \varrho r^3 b_n + r^3 O(L^{-1}) \ . \tag{5.90}$$

Secondly, we have, for all $n\in\mathbb{N}$ and any nonnegative trace-class operator $A$ in $\mathcal{H}^1$, by expanding the trace in a complete set $\{\psi_j\}_{j\in\mathbb{N}}$ of eigenvectors of $A$ with corresponding eigenvalues $\{\lambda_j\}_{j\in\mathbb{N}}$,

$$\int_\Lambda d^3z \ \operatorname{tr}\left(D_{r,z}^{2n} A\right) = \int_\Lambda d^3z \sum_{j\in\mathbb{N}} \lambda_j \int_\Lambda d^3x\, d_r^n(x-z)\,|\,\psi_j(x)\,|^2 = r^3 b_n \operatorname{tr}(A) \ , \tag{5.91}$$

where we have used monotone convergence and Fubini's Theorem. Thus we obtain for the integral of the direct part in (5.76)

$$\int_0^\infty dr\, g(r) \int_\Lambda d^3z \ \operatorname{tr}\left(D_{r,z}^2 \gamma_\omega\right) \operatorname{tr}\left(D_{r,z}^2 P_\mu\right) = b_1^2\,\varrho\, g_6 \ \operatorname{tr}(\gamma_\omega) + \operatorname{tr}(\gamma_\omega)\ O(L^{-1}) \ . \tag{5.92}$$

Similarly, we have for the integral of the direct part in (5.77)

$$\int_0^\infty dr\, g(r) \int_\Lambda d^3z \ \operatorname{tr}\left(D_{r,z}^2 P_\mu\right)^2 = L^3 \varrho^2 b_1^2 g_6 + O(L^2) \ . \tag{5.93}$$

Actually, (5.92) partially cancels $\operatorname{tr}(h_\varrho \gamma)$, see (5.63). Namely:

$$\frac{1}{\lambda}\omega(J_\varrho \cdot \mathbf{1}) = \varrho \operatorname{tr}(\gamma_\omega) \int_\Lambda d^3x \int_0^\infty dr\, g(r) \int_\Lambda d^3z\, d_r(x-z) d_r(z) = b_1^2\,\varrho\, g_6 \operatorname{tr}(\gamma_\omega) \ . \tag{5.94}$$

Hence, we have the following cancellation:

$$(5.92) - (5.94) = O\big(L^{-1}\big)\,\mathrm{tr}\,(\gamma_\omega) \ . \tag{5.95}$$

Taking into account (5.95), (5.76) and (5.77), we obtain from (5.72):

$$\begin{aligned}
\omega\left(H_\varrho\right) &= \mathrm{tr}\,\big((-\triangle - \mu\cdot\mathbf{1})\gamma_\omega\big) \\
&\quad - \lambda \int_0^\infty dr\, g(r) \int_\Lambda d^3z\ \mathrm{tr}\,\big(D_{r,z}^2(\gamma_\omega - P_\mu)D_{r,z}^2 P_\mu\big) \\
&\quad - \frac{\lambda}{2}\int_0^\infty dr\, g(r)\int_\Lambda d^3z\ \mathrm{tr}\,\big(D_{r,z}^2 P_\mu D_{r,z}^2 P_\mu\big) - \frac{\lambda}{2}L^3 g_6 b_1^2 \varrho^2 \\
&\quad + \frac{\lambda}{2}\int_0^\infty dr\, g(r)\int_\Lambda d^3z \sum_{p,q\in\mathbb{N}} \omega\big(:a^*(D_{r,z}f_p)a^*(D_{r,z}f_q)a(D_{r,z}f_q)a(D_{r,z}f_p):_\mu\big) \\
&\quad + O(L^2) + O(L^{-1})\,\mathrm{tr}\,(\gamma_\omega) \ .
\end{aligned} \tag{5.96}$$

If we have $v = v_\nu$, for some $\nu > 0$, then $g$ and $\{d_r\}_{r>0}$ are given by (4.34b). It is then obvious that $g_6$ and $b_1$ are finite. □

### Introducing the Truncated Density Matrix $\gamma^{(t)}$

**Definition 5.8.** *For any chemical potential $\mu > 0$ and any density matrix $\gamma$, we define the truncated density matrix $\gamma^{(t)}$ by*

$$\gamma^{(t)} \ := \ P_\mu(\mathbf{1} - \gamma)P_\mu + P_\mu^\perp \gamma P_\mu^\perp \ . \tag{5.97}$$

The next step we take is to reexpress $T_\mu(\gamma)$ and to estimate $I_\mu^{(1)}(\gamma)$ and $I_\mu^{(2)}$, completely eliminating $\gamma$ in the first two of these cases. Each of these estimates is formulated in a separate lemma.

**Lemma 5.9.** *Let $\gamma$ be an arbitrary density matrix. Then the kinetic energy term $T_\mu(\gamma)$ depends on $\gamma$ just through $\gamma^{(t)}$ and we have*

$$T_\mu(\gamma) = \mathrm{tr}\,\big(|-\triangle - \mu\cdot\mathbf{1}\,|\,\gamma^{(t)}\big) - L^3\frac{2}{5}c_{TF}\varrho^{\frac{5}{3}} + O(L^{-3}) \ , \tag{5.98}$$

*where*

$$c_{TF} := \big(6\pi^2\big)^{\frac{2}{3}} \tag{5.99}$$

*is the Thomas-Fermi constant.*

*Proof:* We note first that

$$[\triangle, P_\mu] = \Big[\triangle, P_\mu^\perp\Big] = \mathbf{0}\restriction_{\mathcal{D}(\triangle)} \ , \tag{5.100}$$

since $P_\mu$ is a spectral projection of $-\triangle$. Secondly, we note that

$$(-\triangle - \mu\cdot\mathbf{1})\restriction_{\mathrm{ran}\,P_\mu} \leq \mathbf{0} \qquad \text{and} \qquad (-\triangle - \mu\cdot\mathbf{1})\restriction_{\mathrm{ran}\,P_\mu^\perp} \geq \mathbf{0} \ . \tag{5.101}$$

We can thus conclude

$$\begin{aligned}
\mathrm{tr}\,\big((-\triangle - \mu\cdot\mathbf{1})\gamma\big) &= \mathrm{tr}\,\Big((-\triangle - \mu\cdot\mathbf{1})\,\Big(P_\mu^\perp\gamma P_\mu^\perp + P_\mu(\gamma - \mathbf{1})P_\mu + P_\mu\Big)\Big) \\
&= \mathrm{tr}\,\big(|-\triangle - \mu\cdot\mathbf{1}\,|\,\gamma^{(t)}\big) + \mathrm{tr}\,\big((-\triangle - \mu\cdot\mathbf{1})P_\mu\big) \ .
\end{aligned}$$

Furthermore, it is easy to verify that

$$\operatorname{tr}\big( (-\Delta - \mu \cdot \mathbf{1})\, P_\mu \big) = -L^3 \frac{2}{5} (6\pi^2)^{\frac{2}{3}} \varrho^{\frac{5}{3}} + O(L^{-3}) \;, \tag{5.102}$$

completing the proof. □

**Lemma 5.10.** *Suppose $v = v_\nu$, for some $\nu > 0$. Then, for large $L$, the expression $I^{(1)}_\mu(\gamma)$ can be asymptotically estimated in terms of $\gamma^{(t)}$ as follows:*

$$I^{(1)}_\mu(\gamma) \leq L^3\, c_2(\delta)\, g_{\frac{8+\delta}{2}} \sqrt{b_2}\, \varrho^{\frac{5+\delta}{6}} \left\{ \sqrt{\frac{\operatorname{tr}(\gamma^{(t)})}{L^3}} + 2 \sqrt[4]{\left(\varrho + \frac{\operatorname{tr}(\gamma^{(t)})}{L^3}\right) \frac{\operatorname{tr}(\gamma^{(t)})}{L^3}} \right\} \;, \tag{5.103}$$

*for any $\delta \in [0,1]$ and all $\mu > 0$. The constant $c_2(\delta)$ is uniformly bounded in $\delta$. Moreover, $g_{\frac{8+\delta}{2}}$ and $b_2$, given in* (5.79)*, are finite.*

*Proof:* For any $\gamma \geq 0$ in $\mathcal{B}(\mathcal{H}^1)$ with $\operatorname{tr}(\gamma) < \infty$, we observe

$$\begin{aligned} I^{(1)}_\mu(\gamma) &= \\ &= \int_0^\infty dr\, g(r) \int_\Lambda d^3z\ \operatorname{tr}\left( D^2_{r,z} \left( P_\mu(\gamma - \mathbf{1})P_\mu + P_\mu^\perp \gamma P_\mu + P_\mu \gamma P_\mu^\perp + P_\mu^\perp \gamma P_\mu^\perp \right) D^2_{r,z} P_\mu \right) \\ &\leq \int_0^\infty dr\, g(r) \int_\Lambda d^3z \left\{ \operatorname{tr}\left( D^2_{r,z} \gamma^{(t)} D^2_{r,z} P_\mu \right) + \operatorname{tr}\left( D^2_{r,z} P_\mu^\perp \gamma P_\mu D^2_{r,z} P_\mu \right) \right. \\ &\qquad \left. + \operatorname{tr}\left( D^2_{r,z} P_\mu \gamma P_\mu^\perp D^2_{r,z} P_\mu \right) \right\} \;. \end{aligned} \tag{5.104}$$

Repeatedly using the Cauchy-Schwarz estimate, yields:

$$\int_\Lambda d^3z\ \operatorname{tr}\left( D^2_{r,z} \gamma^{(t)} D^2_{r,z} P_\mu \right) \leq C \sqrt{\int_\Lambda d^3z\ \operatorname{tr}\left( (D_{r,z} \gamma^{(t)} D_{r,z})^2 \right)} \;, \tag{5.105a}$$

$$\int_\Lambda d^3z\ \operatorname{tr}\left( D^2_{r,z} P_\mu^\perp \gamma P_\mu D^2_{r,z} P_\mu \right) \leq C \sqrt{\int_\Lambda d^3z\ \operatorname{tr}\left( D^2_{r,z} P_\mu^\perp \gamma P_\mu D^2_{r,z} P_\mu \gamma P_\mu^\perp \right)} \;, \tag{5.105b}$$

$$\int_\Lambda d^3z\ \operatorname{tr}\left( D^2_{r,z} P_\mu \gamma P_\mu^\perp D^2_{r,z} P_\mu \right) \leq C \sqrt{\int_\Lambda d^3z\ \operatorname{tr}\left( D^2_{r,z} P_\mu \gamma P_\mu^\perp D^2_{r,z} P_\mu^\perp \gamma P_\mu \right)} \;. \tag{5.105c}$$

The factor $C$ common to all of the three bounds above is given by:

$$C := \sqrt{\int_\Lambda d^3z\ \operatorname{tr}\left( P_\mu D^2_{r,z} P_\mu D^2_{r,z} \right)} \;. \tag{5.106}$$

Since $v = v_\nu$, we can suppose that $g$ and $\{d_r\}_{r>0}$ are of the form (4.34b). Therefore, we can estimate $C$ as follows.

$$\begin{aligned}
C^2 &= \int_\Lambda d^3z \sum_{k,k'\in\Lambda^*_\mu} \left| \left\langle \phi_{k'} \,\middle|\, D^2_{r,z}\phi_k \right\rangle \right|^2 \\
&= \int_\Lambda d^3z \, \frac{1}{L^6} \sum_{k,k'\in\Lambda^*_\mu} \left| \int_{\mathbb{R}^3} d^3x \, e^{i(k-k')x} d\left(\frac{x-z}{r}\right) \right|^2 \\
&= L^3 r^6 \frac{1}{L^6} \sum_{k,k'\in\Lambda^*_\mu} \left| \int_{\mathbb{R}^3} d^3x \, \exp\left(ir(k-k')x - x^2\right) \right|^2 \\
&= \frac{L^3 r^6}{2^6\pi^3} \int_{|k'|\le\sqrt{\mu}} d^3k' \int_{|k|\le\sqrt{\mu}} d^3k \, e^{-\frac{r^2}{2}|k-k'|^2} + O(L^{-3}) \\
&\le \frac{L^3 r^6}{2^6\pi^3} \int_{|k'|\le\sqrt{\mu}} d^3k' \int_{|k|\le 2\sqrt{\mu}} d^3k \, e^{-\frac{r^2}{2}|k|^2} + O(L^{-3}) \\
&= \frac{L^3 r^3}{2^2\cdot 3\pi} \mu^{\frac{3}{2}} \int_0^{2r\sqrt{\mu}} d\kappa \, \kappa^2 e^{-\frac{1}{2}\kappa^2} + O(L^{-3}) \; .
\end{aligned} \tag{5.107}$$

In the first step, we have expanded the trace in terms of the complete orthonormal set $\{\phi_k\}_{k\in\Lambda^*}$ given in (5.67). Subsequently we have used the form of $d$ given in (4.34b). The remaining integral can be estimated as follows: For any $\delta \in (0,1)$, we have:

$$\int_0^{2r\sqrt{\mu}} d\kappa \, \kappa^2 e^{-\frac{1}{2}\kappa^2} \le (2r\sqrt{\mu})^{2+\delta} \int_0^{2r\sqrt{\mu}} \frac{1}{\kappa^\delta} e^{-\frac{1}{2}\kappa^2} \le (2r\sqrt{\mu})^{2+\delta} \int_0^\infty \frac{1}{\kappa^\delta} e^{-\frac{1}{2}\kappa^2} \; . \tag{5.108}$$

Alternatively, we can also estimate the right hand side of this inequality by

$$\int_0^{2r\sqrt{\mu}} d\kappa \, \kappa^2 e^{-\frac{1}{2}\kappa^2} \le \int_0^{2r\sqrt{\mu}} d\kappa \, \kappa^2 = \frac{1}{3}(2r\sqrt{\mu})^3 \; . \tag{5.109}$$

(Note that this estimate leads to the same power law as the previous one in the case $\delta = 1$.) Thus, for all $\delta \in [0,1]$ and sufficiently large $L$, we obtain the estimate:

$$C \le L^{\frac{3}{2}} \, c_2(\delta) \, r^{\frac{5+\delta}{2}} \, \varrho^{\frac{5+\delta}{6}} \; , \tag{5.110}$$

where we have used (5.70). The constant $c_2(\delta)$ is given by

$$c_2(\delta) := \varepsilon + \min\left\{ \sqrt{\frac{2^\delta}{3\pi}(6\pi^2)^{\frac{5+\delta}{3}} \int_0^\infty \frac{1}{\kappa^\delta} e^{-\frac{k^2}{2}}}, (2\pi)^{\frac{3}{2}} \right\} < \infty \; . \tag{5.111}$$

The additional $\varepsilon > 0$ is there to absorb the $O(L^{-\frac{3}{2}})$ appearing in the estimate (5.107). It can be chosen arbitrarily small.

The second factor in (5.105a) is easy to estimate. Namely, we use $\gamma^{(t)} \le \mathbf{1}$ and (5.91) to estimate

$$\sqrt{\int_\Lambda d^3z \; \mathrm{tr}\left((D_{r,z}\gamma^{(t)}D_{r,z})^2\right)} \le \sqrt{\int_\Lambda d^3z \; \mathrm{tr}\left(D^4_{r,z}\gamma^{(t)}\right)} = r^{\frac{3}{2}} \sqrt{b_2} \sqrt{\mathrm{tr}\left(\gamma^{(t)}\right)} \; . \tag{5.112}$$

The estimate of the second factor on the right hand side of (5.105b) is somewhat more complicated. The Cauchy-Schwarz inequality and (5.91) together with $P_\mu \gamma P_\mu \leq \mathbf{1}$ and $P_\mu^\perp \gamma P_\mu^\perp \leq \mathbf{1}$ imply

$$\begin{aligned}
&\int_\Lambda d^3z \ \mathrm{tr}\left(D_{r,z}^2 P_\mu^\perp \gamma P_\mu D_{r,z}^2 P_\mu \gamma P_\mu^\perp\right) \\
&\qquad \leq \sqrt{\int_\Lambda d^3z \ \mathrm{tr}\left(\gamma P_\mu D_{r,z}^2 P_\mu \gamma P_\mu D_{r,z}^2 P_\mu\right)}\sqrt{\int_\Lambda d^3z \ \mathrm{tr}\left(\gamma P_\mu^\perp D_{r,z}^2 P_\mu^\perp \gamma P_\mu^\perp D_{r,z}^2 P_\mu^\perp\right)} \\
&\qquad \leq \sqrt{\int_\Lambda d^3z \ \mathrm{tr}\left(D_{r,z}^4 P_\mu \gamma P_\mu\right)}\sqrt{\int_\Lambda d^3z \ \mathrm{tr}\left(D_{r,z}^4 P_\mu^\perp \gamma P_\mu^\perp\right)} \\
&\qquad = b_2 r^3 \sqrt{\mathrm{tr}\left(P_\mu \gamma\right) \mathrm{tr}\left(P_\mu^\perp \gamma\right)} \\
&\qquad = b_2 r^3 \sqrt{\left(\varrho L^3 + \mathrm{tr}\left(P_\mu(\gamma - \mathbf{1})\right)\right) \mathrm{tr}\left(P_\mu^\perp \gamma\right)} \\
&\qquad \leq L^3 b_2 r^3 \sqrt{\left(\varrho + \frac{\mathrm{tr}\left(\gamma^{(t)}\right)}{L^3}\right)\frac{\mathrm{tr}\left(\gamma^{(t)}\right)}{L^3}} \ .
\end{aligned} \tag{5.113}$$

The estimate of the second factor in (5.105c) is completely analogous, i. e., we have:

$$\int_\Lambda d^3z \ \mathrm{tr}\left(D_{r,z}^2 P_\mu \gamma P_\mu^\perp D_{r,z}^2 P_\mu^\perp \gamma P_\mu\right) \leq L^3 b_2 r^3 \sqrt{\left(\varrho + \frac{\mathrm{tr}\left(\gamma^{(t)}\right)}{L^3}\right)\frac{\mathrm{tr}\left(\gamma^{(t)}\right)}{L^3}} \ . \tag{5.114}$$

Collecting (5.110), (5.112), (5.113) and (5.114) proves the claim. □

**Lemma 5.11.** *Suppose $v = v_\nu$, for some $\nu > 0$. Then, for large $L$, the expression $I_\mu^{(2)}$, see* (5.82)*, can be asymptotically estimated as follows*

$$I_\mu^{(2)} \leq 2 c_D \varrho^{\frac{4}{3}} L^3 + O(L^{-3}) \ , \tag{5.115}$$

*$c_D$ denoting Dirac's constant. It is given by*

$$c_D := \frac{3^{\frac{4}{3}}}{2^{\frac{5}{3}}} \pi^{-\frac{1}{3}} \ . \tag{5.116}$$

*Proof:* In fact, the integral $I_\mu^{(2)}$ can be done explicitly. We obtain:

$$\begin{aligned}
I_\mu^{(2)} &= \int_0^\infty dr\, g(r) \int_\Lambda d^3z \ \mathrm{tr}\left(D_{r,z}^2 P_\mu D_{r,z}^2 P_\mu\right) \\
&= \int_0^\infty dr\, g(r) \int_\Lambda d^3z \sum_{k,k' \in \Lambda_\mu^*} \left| \langle \phi_k \,|\, D_{r,z}^2 \phi_{k'} \rangle \right|^2 \\
&= \int_0^\infty dr\, g(r) \int_\Lambda d^3z \, \frac{1}{L^6} \sum_{k,k' \in \Lambda_\mu^*} \left| \int_{\mathbb{R}^3} d^3x \ \exp\left(-i(k-k')x - \frac{1}{r^2}(x-z)^2\right) \right|^2 \\
&= L^3 \int_0^\infty dr\, g(r) r^6 \frac{1}{L^6} \sum_{k,k' \in \Lambda_\mu^*} \left| \int_{\mathbb{R}^3} d^3x \ \exp\left(-ir(k-k')x - x^2\right) \right|^2 \\
&= \frac{L^3}{2^6 \pi^3} \int_0^\infty dr\, g(r) r^6 \int_{|k| \leq \sqrt{\mu}} d^3k \int_{|k'| \leq \sqrt{\mu}} d^3k' \exp\left(-\frac{r^2}{2} \left| k - k' \right|^2\right) + O(L^{-3}) = \dots
\end{aligned}$$

$$
\begin{aligned}
&= \frac{L^3}{2^6\pi^3} \int_{|\,k\,|\leq\sqrt{\mu}} d^3k \int_{|\,k'\,|\leq\sqrt{\mu}} d^3k' \int_0^\infty dr\, g(r) r^6 \exp\left(-\frac{r^2}{2}\,|\,k-k'\,|^2\right) + O(L^{-3}) \\
&= \frac{L^3}{2^4\pi^5} \int_{|\,k\,|\leq\sqrt{\mu}} d^3k \int_{|\,k'\,|\leq\sqrt{\mu}} d^3k' \frac{2}{\nu^2 + |\,k-k'\,|^2} \int_0^\infty dr\, re^{-r^2} + O(L^{-3}) \\
&= \frac{L^3\mu^2}{2^4\pi^5} \int_{|\,k\,|\leq 1} d^3k \int_{|\,k'\,|\leq 1} d^3k' \frac{1}{\frac{\nu^2}{\mu} + |\,k-k'\,|^2} + O(L^{-3}) \\
&= \frac{L^3\mu^2}{2^3\pi^4} \int_{|\,k\,|\leq 1} d^3k \int_0^1 ds'\,(s')^2 \int_0^\pi d\theta\, \frac{\sin\theta}{\frac{\nu^2}{\mu} + |\,k\,|^2 + (s')^2 - 2\,|\,k\,|\,s'\cos\theta} + O(L^{-3}) \\
&= \frac{L^3\mu^2}{2^4\pi^4} \int_{|\,k\,|\leq 1} d^3k \int_0^1 ds'\, \frac{s'}{|\,k\,|} \ln\left(\frac{\frac{\nu^2}{\mu} + (|\,k\,| + s')^2}{\frac{\nu^2}{\mu} + (|\,k\,| - s')^2}\right) + O(L^{-3}) \\
&= \frac{L^3\mu^2}{2^2\pi^3} \int_0^1 ds\, s \int_0^1 ds'\, s' \ln\left(\frac{\frac{\nu^2}{\mu} + (s+s')^2}{\frac{\nu^2}{\mu} + (s-s')^2}\right) + O(L^{-3})\ . \qquad (5.117)
\end{aligned}
$$

By our choice of $\mu$, see (5.70), we have

$$
I_\mu^{(2)} = 2c_D \varrho^{\frac{4}{3}} L^3 I(\nu) + O(L^{-3})\ , \qquad (5.118)
$$

where we have introduced

$$
I(\nu) := \int_0^1 ds\, s \int_0^1 ds'\, s' \ln\left(\frac{\frac{\nu^2}{\mu} + (s+s')^2}{\frac{\nu^2}{\mu} + (s-s')^2}\right) \quad , \qquad \forall\ \nu \geq 0\ . \qquad (5.119)
$$

The integral $I(\nu)$ can be done explicitly and yields the somewhat cumbersome expression

$$
\begin{aligned}
&\int_0^1 ds\, s \int_0^1 ds'\, s' \ln\left(\frac{\iota^2 + (s+s')^2}{\iota^2 + (s-s')^2}\right) \\
&\qquad = 1 - \frac{1}{24}\left(4\iota^2 + 32\iota \arctan\left(\tfrac{1}{\iota}\right) + \iota^2\left(12 + \iota^2\right) \ln \tfrac{\iota^2}{4+\iota^2}\right)\ , \qquad (5.120)
\end{aligned}
$$

for any real, nonzero $\iota$ (iota, the forgotten letter of the Greek alphabet). In particular it follows that $I(0) = 1$, corresponding to the Coulomb limiting case. In fact, this is the only case we are interested in, since by the very definition of $I_\mu^{(2)}$, it is obvious that

$$
I_\mu^{(2)}|_{\nu=0} \geq I_\mu^{(2)} \quad , \qquad \forall\ \nu \geq 0\ . \qquad (5.121)
$$

This last observation together with (5.118) proves the claim. □

The next task is to estimate the error term $Z_\mu(\omega)$, given in (5.83), in terms of the truncated density matrix associated to the admissible state $\omega$. This is achieved by the following theorem, the proof of which is based on the correlation estimate in Theorem 5.5.

**Theorem 5.12.** *Suppose $v = v_\nu$, for some $\nu > 0$. Then we have the following correlation estimate.*

$$
\begin{aligned}
Z_\mu(\omega) \geq -c_1\, L^3\, \varrho^{\frac{1}{3}} &\left(\frac{\mathrm{tr}\left(\gamma_\omega^{(t)}\right)}{L^3}\right)^{\frac{1}{3}} \left(4\varrho + \frac{\mathrm{tr}\left(\gamma_\omega^{(t)}\right)}{L^3}\right)^{\frac{2}{3}} \\
&+ \frac{\mathrm{tr}\left(\gamma_\omega^{(t)}\right)}{L^3} R\left(\gamma_\omega^{(t)}\right)^2 O(L^2) + R\left(\gamma_\omega^{(t)}\right)^{-1} O(L^2)\ . \qquad (5.122)
\end{aligned}
$$

*Here, $\gamma_\omega^{(t)}$ denotes the truncated density matrix associated to the state $\omega$. The constant $c_1$ and the expression $R\left(\gamma_\omega^{(t)}\right)$ are given by*

$$c_1 := \frac{4}{\pi^2}\frac{3}{2^{\frac{2}{3}}}7^{\frac{1}{3}}(b_1 b_2)^{\frac{2}{3}} \qquad \text{and} \qquad R\left(\gamma_\omega^{(t)}\right) := \sqrt[3]{\frac{1}{\varrho} + 4\frac{L^3}{\mathrm{tr}\left(\gamma_\omega^{(t)}\right)}} \ . \tag{5.123}$$

*Proof:* We recall Theorem 5.5. In the present context, we have

$$w = w_\mu = \begin{pmatrix} P_\mu^\perp & P_\mu \\ P_\mu & P_\mu^\perp \end{pmatrix} , \tag{5.124}$$

with $P_\mu$ given by (5.71). Therefore, $\tilde{\gamma}$, given in (5.24), satisfies

$$\tilde{\gamma} = P_\mu^\perp \gamma_\omega P_\mu^\perp + P_\mu \alpha_\omega^* P_\mu^\perp + P_\mu^\perp \alpha_\omega P_\mu + P_\mu \left(\mathbf{1} - \bar{\gamma}_\omega\right) P_\mu \ . \tag{5.125}$$

If we insert this into (5.23), several terms vanish due to the fact that $P_\mu P_\mu^\perp = P_\mu^\perp P_\mu = \mathbf{0}$. We obtain

$$\begin{aligned}\sum_{p,q\in\mathbb{N}} \omega\left(:a_p^* a_q^* a_q a_p:_\mu\right) \geq& -4\,\mathrm{tr}\left(D_{r,z}^2 P_\mu^\perp \gamma P_\mu^\perp\right)\mathrm{tr}\left(D_{r,z}^2 P_\mu\right) \\ &- 4\,\mathrm{tr}\left(D_{r,z}^2 P_\mu\right)\sqrt{\mathrm{tr}\left(D_{r,z}^2 P_\mu(\mathbf{1}-\gamma)P_\mu\right)\mathrm{tr}\left(D_{r,z}^2 P_\mu^\perp \gamma P_\mu^\perp\right)} \\ &- 2\sqrt{\mathrm{tr}\left(D_{r,z}^2 P_\mu^\perp \gamma P_\mu^\perp\right)\mathrm{tr}\left(D_{r,z}^2 P_\mu\right)}\Big[\mathrm{tr}\left(D_{r,z}^2 P_\mu \gamma P_\mu D_{r,z}^2 P_\mu^\perp\right) \\ &\qquad + \mathrm{tr}\left(D_{r,z}^2 P_\mu^\perp \gamma P_\mu^\perp\right)\mathrm{tr}\left(D_{r,z}^2 P_\mu\right)\Big]^{\frac{1}{2}} ,\end{aligned} \tag{5.126}$$

where we have used the abbreviation

$$a_p^\sigma := a^\sigma(D_{r,z} f_p) \quad , \qquad \forall\, p\in\mathbb{N},\ \sigma\in\{\varnothing, *\} \ . \tag{5.127}$$

By the definition of $\gamma_\omega^{(t)}$, see (5.97), we can estimate $P_\mu^\perp \gamma_\omega P_\mu^\perp \leq \gamma_\omega^{(t)}$ and $P_\mu(\mathbf{1}-\gamma_\omega)P_\mu \leq \gamma_\omega^{(t)}$. Furthermore, $\gamma \leq \mathbf{1}$. Hence, we can estimate

$$\begin{aligned}\sum_{p,q\in\mathbb{N}} \omega\left(:a_p^* a_q^* a_q a_p:_\mu\right) \geq& -8\,\mathrm{tr}\left(D_{r,z}^2 \gamma_\omega^{(t)}\right)\mathrm{tr}\left(D_{r,z}^2 P_\mu\right) \\ &- 2\sqrt{\mathrm{tr}\left(D_{r,z}^2 \gamma_\omega^{(t)}\right)\mathrm{tr}\left(D_{r,z}^2 P_\mu\right)}\sqrt{\mathrm{tr}\left(D_{r,z}^2 P_\mu D_{r,z}^2 P_\mu^\perp\right) + \mathrm{tr}\left(D_{r,z}^2 \gamma_\omega^{(t)}\right)\mathrm{tr}\left(D_{r,z}^2 P_\mu\right)} \ .\end{aligned} \tag{5.128}$$

Since $x\in\mathbb{R}^+ \mapsto \sqrt{x}$ is sub-additive, we obtain

$$\begin{aligned}\sum_{p,q\in\mathbb{N}} \omega\left(:a_p^* a_q^* a_q a_p:_\mu\right) \geq& -10\,\mathrm{tr}\left(D_{r,z}^2 \gamma_\omega^{(t)}\right)\mathrm{tr}\left(D_{r,z}^2 P_\mu\right) \\ &- 2\sqrt{\mathrm{tr}\left(D_{r,z}^2 \gamma_\omega^{(t)}\right)\mathrm{tr}\left(D_{r,z}^2 P_\mu\right)\mathrm{tr}\left(D_{r,z}^2 P_\mu D_{r,z}^2\right)} ,\end{aligned} \tag{5.129}$$

where we have also dropped the last remaining $P_\mu^\perp$. Next, we use the elementary estimate

$$2ab \leq \varepsilon a^2 + \frac{1}{\varepsilon}b^2 \quad , \qquad \forall\, a,b\in\mathbb{R},\ \varepsilon > 0 \ , \tag{5.130}$$

to conclude, for any strictly positive function $\varepsilon : \mathbb{R}^+ \to \mathbb{R}^+$,

$$\sum_{p,q\in\mathbb{N}} \omega\left(:a_p^* a_q^* a_q a_p:_\mu\right) \geq -\big(10+\varepsilon(r)\big)\, \mathrm{tr}\left(D_{r,z}^2 \gamma_\omega^{(t)}\right) \mathrm{tr}\left(D_{r,z}^2 P_\mu\right) - \frac{1}{\varepsilon(r)}\, \mathrm{tr}\left(D_{r,z}^4 P_\mu\right)\ , \tag{5.131}$$

for all $r > 0$. We now carry out the integration over $z \in \Lambda$. This yields, using (5.90) and (5.91),

$$\begin{aligned}\int_\Lambda d^3z \sum_{p,q\in\mathbb{N}} \omega\big(:a^*(D_{r,z}f_p)a^*(D_{r,z}f_q)a(D_{r,z}f_q)a(D_{r,z}f_p):_\mu\big) \geq \\ -\big(10+\varepsilon(r)\big) r^6 b_1^2 \varrho\, \mathrm{tr}\left(\gamma_\omega^{(t)}\right) - \frac{1}{\varepsilon(r)} L^3 r^3 b_2 \varrho \\ + \big(10+\varepsilon(r)\big) r^6\, \mathrm{tr}\left(\gamma_\omega^{(t)}\right) O(L^{-1}) + \frac{1}{\varepsilon(r)} r^3 O(L^2)\ .\end{aligned} \tag{5.132}$$

The following lemma provides another, simpler correlation estimate, which we use to improve the above estimate for large $r$. We postpone the proof of this lemma until after the end of the current proof (see page 115).

**Lemma 5.13.** *Suppose $v = v_\nu$, for some $\nu > 0$. We denote by $\gamma_\omega^{(t)}$ the truncated density matrix of the admissible state $\omega$ and additionally we assume that its two-particle density matrix is trace-class. Then we have the following estimate:*

$$\begin{aligned}\int_\Lambda d^3z \sum_{p,q\in\mathbb{N}} \omega\big(:a^*(D_{r,z}f_p)a^*(D_{r,z}f_q)a(D_{r,z}f_q)a(D_{r,z}f_p):_\mu\big) \\ \geq -r^3\, b_2 \Big(\mathrm{tr}\left(\gamma_\omega^{(t)}\right) + 2\varrho L^3\Big) + r^3 O(L^2)\ .\end{aligned} \tag{5.133}$$

We now use the correlation estimate (5.132) for small values of the length scale parameter $r$ and the correlation estimate (5.133) for large values of $r$, to obtain the following combined estimate:

$$\begin{aligned}\int_0^\infty dr\, g(r) \int_\Lambda d^3z \sum_{p,q\in\mathbb{N}} \omega\big(:a^*(D_{r,z}f_p)a^*(D_{r,z}f_q)a(D_{r,z}f_q)a(D_{r,z}f_p):_\mu\big) \\ \geq -\int_0^R dr\, g(r) \Big\{ \big(10+\varepsilon(r)\big) b_1^2 \varrho r^6\, \mathrm{tr}\left(\gamma_\omega^{(t)}\right) \\ + \big(10+\varepsilon(r)\big) r^6\, \mathrm{tr}\left(\gamma_\omega^{(t)}\right) O(L^{-1}) + \frac{1}{\varepsilon(r)} L^3 r^3 b_2 \varrho + \frac{1}{\varepsilon(r)} r^3 O(L^2) \Big\} \\ - \int_R^\infty dr\, g(r) r^3 b_2 \left(\mathrm{tr}\left(\gamma_\omega^{(t)}\right) + 2\varrho L^3 + O(L^2)\right)\ ,\end{aligned} \tag{5.134}$$

for any $R > 0$. Since $v = v_\nu$, we have

$$g(r) = \frac{4}{\pi^2} \frac{e^{-\frac{1}{2}\nu^2 r^2}}{r^5} \leq \frac{4}{\pi^2} \frac{1}{r^5}\quad ,\qquad \forall\, r > 0\ . \tag{5.135}$$

Let us choose $\varepsilon(r) := (R/r)^{\frac{3}{2}}$, thus ensuring that all the above integrals are finite. We readily obtain the following bound:

$$\begin{aligned}\frac{\pi^2}{4}\int_0^\infty dr\, g(r)\int_\Lambda d^3z \sum_{p,q\in\mathbb{N}} \omega\Big(:a^*(D_{r,z}f_p)a^*(D_{r,z}f_q)a(D_{r,z}f_q)a(D_{r,z}f_p):_\mu\Big) \\ \geq -7\,b_1^2\,\varrho\,\mathrm{tr}\left(\gamma_\omega^{(t)}\right)R^2 - 2\,\varrho\,L^3 b_2\,R^{-1} - b_2\Big(\mathrm{tr}\left(\gamma_\omega^{(t)}\right)+2\varrho L^3\Big)R^{-1} \\ +\,\mathrm{tr}\left(\gamma_\omega^{(t)}\right)R^2 O(L^{-1}) + R^{-1}O(L^2)\ . \end{aligned} \tag{5.136}$$

The next step is to choose the value of $R$ such that the right hand side of (5.136) becomes maximal. Except for the asymptotic error terms, we must maximize a function $f$ of the type

$$f(R) = -aR^2 - \frac{b}{R} \quad , \qquad \forall\, R>0\ . \tag{5.137}$$

In the present case, the nonnegative constants $a$ and $b$ are given by

$$a := 7\,b_1^2\,\varrho\,\mathrm{tr}\left(\gamma_\omega^{(t)}\right) \qquad \text{and} \qquad b := 2\varrho L^3 b_2 + \mathrm{tr}\left(\gamma_\omega^{(t)}\right)b_2 + 2\varrho L^3 b_2\ . \tag{5.138}$$

The value of $R$, where $f$ attains its maximum, is easily seen to be:

$$\tilde{R}(\gamma_\omega^{(t)}) := \sqrt[3]{\frac{b}{2a}} = \sqrt[3]{\frac{L^3}{\mathrm{tr}\left(\gamma_\omega^{(t)}\right)}\cdot\frac{b_2}{b_1^2}\cdot\frac{\frac{\mathrm{tr}\left(\gamma_\omega^{(t)}\right)}{L^3}\varrho^{-1}+4}{14}}\ . \tag{5.139}$$

This leads to the following expression for the maximal value of $f$:

$$f(R)\leq f\left(\tilde{R}\left(\gamma_\omega^{(t)}\right)\right) = -\frac{3}{2^{\frac{2}{3}}}b^{\frac{2}{3}}a^{\frac{1}{3}} \quad , \qquad \forall\, R>0 \tag{5.140}$$

Reinserting this into (5.136), leads to the following estimate of $Z_\mu(\omega)$, see (5.83),

$$\begin{aligned} Z_\mu(\omega) \geq -c_1 L^3\varrho^{\frac{1}{3}}\left(\frac{\mathrm{tr}\left(\gamma_\omega^{(t)}\right)}{L^3}\right)^{\frac{1}{3}}\left(4\varrho+\frac{\mathrm{tr}\left(\gamma_\omega^{(t)}\right)}{L^3}\right)^{\frac{2}{3}} \\ +\frac{\mathrm{tr}\left(\gamma_\omega^{(t)}\right)}{L^3}\tilde{R}\left(\gamma_\omega^{(t)}\right)^2 O(L^2) + \tilde{R}\left(\gamma_\omega^{(t)}\right)^{-1}O(L^2)\ , \end{aligned} \tag{5.141}$$

where we have set

$$c_1 := \frac{4}{\pi^2}\frac{3}{2^{\frac{2}{3}}}7^{\frac{1}{3}}(b_1 b_2)^{\frac{2}{3}}\ . \tag{5.142}$$

Finally, we remark: Even though $b_2$ depends on $L$, we can use the explicit form of $d$, given by (4.34b), to show that $b_2$ is a monotone nonincreasing function of $L$, always larger than some positive constant. Since $b_1$ is independent of $L$, we can thus replace $\tilde{R}\left(\gamma_\omega^{(t)}\right)$ with $R\left(\gamma_\omega^{(t)}\right)$ given in (5.123). $\square$

*Proof of Lemma 5.13:* We use Corollary 5.4 to carry out the normal-ordering prescription in (5.83) directly. This yields, using the shorthand notation (5.127),

$$\begin{aligned}\sum_{p,q\in\mathbb{N}}\omega(:a_p^*a_q^*a_qa_p:_\mu) = \sum_{p,q\in\mathbb{N}}\Big\{\omega(a_p^*a_q^*a_qa_p) - 2\omega(a_p^*a_p)\Omega_\mu(a_q^*a_q) \\ +\,\Omega_\mu(a_p^*a_p)\Omega_\mu(a_q^*a_q) + 2\omega(a_p^*a_q)\Omega_\mu(a_q^*a_p) - \Omega_\mu(a_p^*a_q)\Omega_\mu(a_q^*a_p)\Big\}\ . \end{aligned} \tag{5.143}$$

(Note that in the present context $\Omega_\mu(a_p^* a_q^*) = \Omega_\mu(a_p a_q) = 0$, for all $p$ and $q$ in $\mathbb{N}$.) Furthermore, we may deduce, by performing two anti-commutations and subsequently completing a square resulting from the quartic expectation value,

$$\begin{aligned}\sum_{p,q\in\mathbb{N}} \omega(:a_p^* a_q^* a_q a_p:_\mu) &= \omega\Big( \Big[\sum_{q\in\mathbb{N}} a_q^* a_q - \Omega_\mu(a_q^* a_q)\Big]\Big[\sum_{q\in\mathbb{N}} a_q^* a_q - \Omega_\mu(a_q^* a_q)\Big]^* \Big) \\ &+ \sum_{p,q\in\mathbb{N}} \Big\{ -\left\{a_p^*, a_q\right\} \omega(a_q^* a_p) + 2\omega(a_p^* a_q)\Omega_\mu(a_q^* a_p) - \Omega_\mu(a_p^* a_q)\Omega_\mu(a_q^* a_p) \Big\} \ . \qquad (5.144)\end{aligned}$$

We use the following explicit forms for the remaining expectation values and anti-commutators (see also page 102)

$$\left\{a_p^*, a_q\right\} = \langle f_q \,|\, D_{r,z}^2 f_p \rangle \ , \qquad (5.145)$$

$$\omega(a_p^* a_q) = \langle f_q \,|\, D_{r,z} \gamma D_{r,z} f_p \rangle \ , \qquad (5.146)$$

$$\Omega_\mu(a_p^* a_q) = \langle f_q \,|\, D_{r,z} P_\mu D_{r,z} f_p \rangle \ , \qquad (5.147)$$

for all $p$ and $q$. Simply dropping the positive square and estimating $P_\mu \leq \mathbf{1}$ then yields

$$\begin{aligned}\sum_{p,q\in\mathbb{N}} \omega(:a_p^* a_q^* a_q a_p:_\mu) &\geq -\operatorname{tr}\left(D_{r,z}^4 \gamma\right) + 2\operatorname{tr}\left(D_{r,z}^2 \gamma D_{r,z}^2 P_\mu\right) - \operatorname{tr}\left(D_{r,z}^2 P_\mu D_{r,z}^2 P_\mu\right) \\ &\geq -\operatorname{tr}\left(D_{r,z}^4 \gamma\right) - \operatorname{tr}\left(D_{r,z}^4 P_\mu\right) \ . \qquad (5.148)\end{aligned}$$

Thus we obtain, by (5.91) and (5.90)

$$\int_\Lambda d^3 z \sum_{p,q\in\mathbb{N}} \omega(:a_p^* a_q^* a_q a_p:_\mu) \geq -r^3 b_2 \left(\operatorname{tr}(\gamma) + \varrho L^3 + O(L^2)\right) \ . \qquad (5.149)$$

From here we arrive at the claimed relation by observing

$$\begin{aligned}\operatorname{tr}(\gamma) &= -\operatorname{tr}\left(P_\mu(\mathbf{1}-\gamma)\right) + \operatorname{tr}\left(P_\mu^\perp \gamma\right) + \operatorname{tr}(P_\mu) \\ &\leq \operatorname{tr}\left(\gamma^{(t)}\right) + \operatorname{tr}(P_\mu) = \operatorname{tr}\left(\gamma^{(t)}\right) + \varrho L^3 + O(L^2) \ , \qquad (5.150)\end{aligned}$$

where we have used (5.89). This completes the proof. □

To close this subsection, we summarize: By Lemmas 5.6, 5.9, 5.10, 5.11 and by Theorem 5.12, we have the following theorem.

**Theorem 5.14.** *Suppose $v = v_\nu$, for some $\nu > 0$, and let $\omega$ be an admissible state with the additional property that its two-particle density matrix is trace-class. Then, for any* *density $\varrho > 0$, we have*

$$
\begin{aligned}
\omega\left(H_\varrho\right) \geq & - L^3 \frac{2}{5} c_{TF}\, \varrho^{\frac{5}{3}} + \operatorname{tr}\left( \left| -\triangle - \mu \cdot \mathbf{1} \right| \gamma_\omega^{(t)} \right) \\
& - \lambda L^3 c_2(\delta)\, g_{\frac{8+\delta}{2}} \sqrt{b_2}\, \varrho^{\frac{5+\delta}{6}} \left\{ \sqrt{\frac{\operatorname{tr}\left(\gamma_\omega^{(t)}\right)}{L^3}} + 2 \sqrt[4]{\left( \varrho + \frac{\operatorname{tr}\left(\gamma_\omega^{(t)}\right)}{L^3} \right) \frac{\operatorname{tr}\left(\gamma_\omega^{(t)}\right)}{L^3}} \right\} \\
& - \lambda L^3 c_D\, \varrho^{\frac{4}{3}} \\
& - \frac{\lambda}{2} L^3 g_6\, b_1^2\, \varrho^2 - \frac{\lambda}{2} c_1 L^3 \varrho^{\frac{1}{3}} \left( \frac{\operatorname{tr}\left(\gamma_\omega^{(t)}\right)}{L^3} \right)^{\frac{1}{3}} \left( 4\varrho + \frac{\operatorname{tr}\left(\gamma_\omega^{(t)}\right)}{L^3} \right)^{\frac{2}{3}} \\
& + \frac{\operatorname{tr}\left(\gamma_\omega^{(t)}\right)}{L^3} R\left(\gamma_\omega^{(t)}\right)^2 O(L^2) + \left( R\left(\gamma_\omega^{(t)}\right)^{-1} + 1 \right) O(L^2) + \operatorname{tr}\left(\gamma_\omega^{(t)}\right) O(L^{-1}) \ . \qquad (5.151)
\end{aligned}
$$

*Here, $\mu = \left(6\pi^2 \varrho\right)^{\frac{2}{3}}$ and the constants $c_{TF}$, $c_1$, $c_2(\delta)$ and $c_D$ are given in* (5.99), (5.142), (5.111), (5.132). *$\delta \in [0,1]$ is arbitrary. The expression $R(\gamma_\omega^{(t)})$ is given in* (5.123).

### Minimizing in $\gamma_\omega^{(t)}$

We proceed estimating $\omega\left(H_\varrho\right)$ by viewing the right hand side of (5.151) as a function of $\gamma_\omega^{(t)}$ and by minimizing this function. To emphasize this change of perspective, we shall from now on write $\gamma^{(t)}$ instead of $\gamma_\omega^{(t)}$, demanding

$$
\gamma^{(t)} \in \mathcal{B}(\mathcal{H}^1) \ , \qquad \mathbf{0} \leq \gamma^{(t)} \leq \mathbf{1} \ , \qquad \operatorname{tr}\left(\gamma^{(t)}\right) < \infty \ . \tag{5.152}
$$

Note that $\gamma_\omega^{(t)}$ satisfies these conditions. It is not obvious that the right hand side of (5.151) possesses a minimizer. However, if there exists a minimizer $\gamma_*^{(t)}$, then $\gamma_*^{(t)}$ also minimizes the function $f$

$$
f\left(\gamma^{(t)}\right) := \operatorname{tr}\left( \left| -\triangle - \mu \cdot \mathbf{1} \right| \gamma^{(t)} \right) \tag{5.153}
$$

under the constraint

$$
\operatorname{tr}\left(\gamma^{(t)}\right) = \bar{\varrho} L^3 \ , \quad \text{with} \qquad \bar{\varrho} := \frac{\operatorname{tr}\left(\gamma_*^{(t)}\right)}{L^3} \ . \tag{5.154}
$$

This motivates us to consider the following family $\{p_\sigma\}_{\sigma \geq 0}$ of truncated density matrices. For any <u>filling parameter</u> $\sigma \geq 0$, we introduce the finite index set

$$
I_\sigma := \left\{ k \in \Lambda^* \ \middle| \ \sqrt{\mu\left(\max\{0, 1-\sigma\}\right)} < |\,k\,| < \sqrt{\mu\,(1+\sigma)} \right\} \ . \tag{5.155}
$$

We define $p_\sigma$ to be the orthogonal projection in $\mathcal{H}^1$ onto the subspace spanned by $\{\phi_k\}_{k \in I_\sigma}$. Namely, we set

$$
p_\sigma \phi_k := \begin{cases} \phi_k & \text{if } k \in I_\sigma \\ 0 & \text{else} \end{cases} \ , \qquad \forall\, \sigma \geq 0,\ k \in \Lambda^* \ , \tag{5.156}
$$

and extend $p_\sigma$ to $\mathcal{H}^1$ by linearity. We recall the definition of $\{\phi_k\}_{k \in \Lambda^*}$ given in (5.67). Figure 5.1 illustrates the definition of $p_\sigma$. The following two lemmas allow us to estimate the right hand side of (5.151) in terms of the filling parameter $\sigma$.

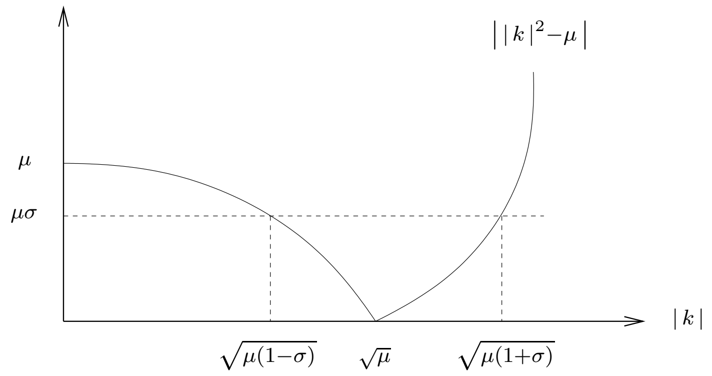


Figure 5.1: The figure shows the graph of the mapping $s \in \mathbb{R} \mapsto \big| s^2 - \mu \big|$. $p_\sigma$ has all its modes $k \in \Lambda^*$ with $\big| |k|^2 - \mu \big|$ smaller than $\sigma \cdot \mu$ filled, while all the rest is empty. Clearly, the behavior of $\mathrm{tr}\,(p_\sigma)$ as a function of $\sigma$ changes at $\sigma = 1$ (corresponding to $\bar{\varrho} = 4\varrho$).

**Lemma 5.15.** *For any density $\varrho > 0$ and any $\bar{\varrho} \geq 0$, we set*

$$\sigma := \begin{cases} \bar{\varrho}\,(4\varrho)^{-1} & , \textit{ for } \ \bar{\varrho} < 4\varrho \\ 2\,\bar{\varrho}^{\frac{2}{3}}\,(4\varrho)^{-\frac{2}{3}} - 1 & , \textit{ for } \ \bar{\varrho} \geq 4\varrho \end{cases} . \tag{5.157}$$

*Then the truncated density matrix $p_\sigma$ defined in* (5.156) *obeys*

$$\frac{\mathrm{tr}\,(p_\sigma)}{L^3} \leq \bar{\varrho} + O(L^{-1}) \ . \tag{5.158}$$

*Furthermore, for any $\gamma^{(t)}$ satisfying* (5.152) *and* $\mathrm{tr}\,(\gamma^{(t)}) = \bar{\varrho} L^3$, *we have*

$$\mathrm{tr}\left(|-\triangle - \mu \cdot \mathbf{1}\,|\,\gamma^{(t)}\right) \geq \mathrm{tr}\left(\,|-\triangle - \mu \cdot \mathbf{1}\,|\,p_\sigma\right) + \sigma\, O(L^2) \ . \tag{5.159}$$

*Proof:* We proceed to prove (5.158). We distinguish two cases.

Case $\bar{\varrho} < 4\varrho$: First note that $0 \leq \sigma < 1$ is implied. We may hence estimate:

$$\begin{aligned} \frac{\mathrm{tr}\,(p_\sigma)}{L^3} &= \frac{1}{2\pi^2} \int_{\sqrt{\mu(1-\sigma)}}^{\sqrt{\mu(1+\sigma)}} ds\, s^2 + O(L^{-1}) \\ &= \varrho \left( (1+\sigma)^{\frac{3}{2}} - (1-\sigma)^{\frac{3}{2}} \right) + O(L^{-1}) \\ &\leq \varrho \left( (1+\sigma)^2 - (1-\sigma)^2 \right) + O(L^{-1}) = 4\varrho\sigma + O(L^{-1}) \ , \end{aligned} \tag{5.160}$$

where we have used (5.70). This proves (5.158), since we have $\sigma = \bar{\varrho}\,(4\varrho)^{-1}$.

Case $\bar{\varrho} \geq 4\varrho$: First note that $\sigma \geq 1$ is implied. We may hence estimate:

$$\begin{aligned} \frac{\mathrm{tr}\,(p_\sigma)}{L^3} = \frac{1}{2\pi^2} \int_0^{\sqrt{\mu(1+\sigma)}} ds\, s^2 + O(L^{-1}) &= \varrho (1+\sigma)^{\frac{3}{2}} + O(L^{-1}) \\ &\leq 4\varrho \left( \frac{1+\sigma}{2} \right)^{\frac{3}{2}} + O(L^{-1}) \ , \end{aligned} \tag{5.161}$$

where we have used (5.70). This proves (5.158), since we have $\sigma = 2\bar{\varrho}^{\frac{2}{3}}(4\varrho)^{-\frac{2}{3}} - 1$.

We have thus proved (5.158), for any $\bar{\varrho} \geq 0$.

We proceed to prove (5.159). To this end, let $\gamma^{(t)}$ have the properties stated in the hypothesis and observe

$$\gamma_k^{(t)} := \left\langle \phi_k \,\middle|\, \gamma^{(t)} \phi_k \right\rangle \ \in \ [0,1] \quad , \qquad \forall\, k \in \Lambda^* \ , \tag{5.162}$$

where $\{\phi_k\}_{k\in\Lambda^*}$ denotes the orthonormal basis introduced in (5.67). Expanding the trace in this basis, we can estimate:

$$\begin{aligned}
\operatorname{tr}\Big( \,|-\triangle - \mu \cdot \mathbf{1}\,|\, \big(\gamma^{(t)} - p_\sigma\big) \Big) &= \sum_{k\in I_\sigma} \Big|\, |\,k\,|^2 - \mu \,\Big| \,\big(\gamma_k^{(t)} - 1\big) + \sum_{k\in\Lambda^*\setminus I_\sigma} \Big|\, |\,k\,|^2 - \mu \,\Big|\, \gamma_k^{(t)} \\
&\geq \mu\sigma \sum_{k\in I_\sigma} \big(\gamma_k^{(t)} - 1\big) + \mu\sigma \sum_{k\in\Lambda^*\setminus I_\sigma} \gamma_k^{(t)} \\
&= \mu\sigma \left( \operatorname{tr}\big(\gamma^{(t)}\big) - \operatorname{tr}\left(p_\sigma\right)\right) \ .
\end{aligned}$$

Using (5.158) and $\operatorname{tr}(\gamma^{(t)}) = \bar{\varrho} L^3$ completes the proof. □

In order to estimate the right hand side of (5.151) entirely in terms of the filling parameter, we must must correspondingly estimate the kinetic term

$$\operatorname{tr}\left( |-\triangle - \mu \cdot \mathbf{1}\,|\, \gamma_\omega^{(t)} \right) \ . \tag{5.163}$$

This is achieved by (5.159) and the following lemma.

**Lemma 5.16.** *For any $\sigma \geq 0$, we have*

$$\operatorname{tr}\Big( \,|-\triangle - \mu \cdot \mathbf{1}\,|\, p_\sigma \Big) \ \geq \ c_3 L^3 \varrho^{\frac{5}{3}} \sigma^2 + O(L^2) \ , \qquad \textit{with} \qquad c_3 := \frac{3}{2^{\frac{3}{2}}} c_{TF} \ . \tag{5.164}$$

*The constant $c_{TF}$ is given in* (5.99).

*Proof:* Again, we distinguish the cases $\sigma < 1$ and $1 \leq \sigma$.

<u>Case $\sigma < 1$:</u> By the definition of $p_\sigma$, we have

$$\begin{aligned}
\operatorname{tr}\big( \,|-\triangle - \mu \cdot \mathbf{1}\,|\, p_\sigma \big) &= \frac{L^3}{2\pi^2} \int_{\sqrt{\mu(1-\sigma)}}^{\sqrt{\mu(1+\sigma)}} ds\, s^2 \,\big|\, s^2 - \mu \,\big| + O(L^2) \\
= \frac{L^3}{2\pi^2} \int_{\sqrt{\mu(1-\sigma)}}^{\sqrt{\mu}} ds\, (s^4 - s^2\mu) &+ \frac{L^3}{2\pi^2} \int_{\sqrt{\mu}}^{\sqrt{\mu(1+\sigma)}} ds\, (s^2\mu - s^4) + O(L^2) \\
= L^3 \frac{\mu^{\frac{5}{2}}}{2\pi^2} \left\{ \frac{4}{15} + \frac{1}{5}(1+\sigma)^{\frac{5}{2}} \right. &\left. - \frac{1}{3}(1+\sigma)^{\frac{3}{2}} - \frac{1}{3}(1-\sigma)^{\frac{3}{2}} + \frac{1}{5}(1-\sigma)^{\frac{5}{2}} \right\} + O(L^2) \ .
\end{aligned} \tag{5.165}$$

The expression in the curly braces can be estimated by

$$\{\ldots\} \geq 2^{-\frac{3}{2}} \sigma^2 \quad , \qquad \forall\, \sigma \in [0,1] \ , \tag{5.166}$$

since we have $\{\dots\}|_{\sigma=0} = 0$ and

$$\frac{d}{d\sigma}\{\dots\} = \frac{1}{2}\Big((1+\sigma)^{\frac{3}{2}} - (1+\sigma)^{\frac{1}{2}} + (1-\sigma)^{\frac{1}{2}} - (1-\sigma)^{\frac{3}{2}}\Big)$$
$$= \frac{\sigma}{2}\Big((1+\sigma)^{\frac{1}{2}} + (1-\sigma)^{\frac{1}{2}}\Big) \geq \frac{\sigma}{\sqrt{2}}\ , \tag{5.167}$$

for[1] all $\sigma$ in $[0,1]$. Integrating (5.167) yields (5.166). Using (5.70), we obtain:

$$\mathrm{tr}\left(|-\triangle - \mu\cdot\mathbf{1}|\,\gamma^{(t)}{}_*\right) \geq c_3\, L^3 \varrho^{\frac{5}{3}}\, \sigma^2 + O(L^2)\ , \qquad \text{with} \qquad c_3 := \frac{(6\pi^2)^{\frac{5}{3}}}{2^{\frac{5}{2}}\pi^2}\ , \tag{5.168}$$

for all $\sigma \in [0,1]$. This completes the proof of the first case.

<u>Case $\sigma \geq 1$:</u>

$$\mathrm{tr}\left(|-\triangle - \mu\cdot\mathbf{1}|\,\gamma^{(t)}{}_*\right) = \frac{L^3}{2\pi^2}\int_0^{\sqrt{\mu(1+\sigma)}} ds\, s^2\, \big|\, s^2 - \mu\, \big| + O(L^2)$$
$$= L^3\frac{\mu^{\frac{5}{2}}}{2\pi^2}\left\{\frac{4}{15} + \frac{1}{5}(1+\sigma)^{\frac{5}{2}} - \frac{1}{3}(1+\sigma)^{\frac{3}{2}}\right\} + O(L^2)\ . \tag{5.169}$$

Again, the expression in the curly braces in (5.169) can be estimated by

$$\{\dots\} \geq 2^{-\frac{3}{2}}\sigma^2 \quad , \qquad \forall\, \sigma \in [1,\infty)\ , \tag{5.170}$$

since we have $\{\dots\}|_{\sigma=1} \geq 2^{-\frac{3}{2}}$ by (5.166) and

$$\frac{d}{d\sigma}\{\dots\} = \frac{1}{2}\Big((1+\sigma)^{\frac{3}{2}} - (1+\sigma)^{\frac{1}{2}}\Big) = \frac{1}{2}(1+\sigma)^{\frac{1}{2}}\sigma \geq \frac{\sigma}{\sqrt{2}}\ , \tag{5.171}$$

for all $\sigma \in [1,\infty)$. Integrating (5.171) yields (5.170). Using (5.70), we obtain again

$$\mathrm{tr}\left(|-\triangle - \mu\cdot\mathbf{1}|\,\gamma^{(t)}{}_*\right) \geq c_3 L^3 \varrho^{\frac{5}{3}}\sigma^2 + O(L^2)\ , \qquad \text{with} \qquad c_3 := \frac{(6\pi^2)^{\frac{5}{3}}}{2^{\frac{5}{2}}\pi^2}\ , \tag{5.172}$$

for all $\sigma \geq 1$. This completes the proof in the second case.

Recall the definition of the Thomas-Fermi constant in (5.99). □

We are now in the position to estimate $\omega(H_\varrho)$ in terms of the filling parameter, as follows.

**Theorem 5.17.** *Suppose $v = v_\nu$, for some $\nu > 0$, and let $\omega$ be an admissible state with the additional property that its two-particle density matrix is trace-class. Furthermore, let $\varrho > 0$ and $\lambda > 0$ be given and set*

$$\bar\varrho := \frac{\mathrm{tr}\left(\gamma_\omega^{(t)}\right)}{L^3} \qquad \textit{and} \qquad \sigma := \begin{cases} \bar\varrho\,(4\varrho)^{-1} & ,\ \textit{for}\ \ \bar\varrho < 4\varrho \\ 2\,\bar\varrho^{\frac{2}{3}}\,(4\varrho)^{-\frac{2}{3}} - 1 & ,\ \textit{for}\ \ \bar\varrho \geq 4\varrho \end{cases}\ . \tag{5.173}$$

[1]Note that in the last step we have estimated the strictly nonincreasing function $(1+\sigma)^{\frac{1}{2}} + (1-\sigma)^{\frac{1}{2}}$ from below by the constant $\sqrt{2}$, which may seem sub-optimal for small values of $\sigma$. However, this simple bound has the correct behavior at $\sigma \sim 0$ as the right and the left hand side together with their derivatives have the same values at $\sigma = 0$.

*Then we have*

$$
\begin{aligned}
\omega\left(H_{\varrho}\right) \geq & - L^3 \frac{2}{5} c_{TF} \varrho^{\frac{5}{3}} + c_3 L^3 \varrho^{\frac{5}{3}} \sigma^2 \\
& - \lambda L^3 c_2(\delta)\, g_{\frac{8+\delta}{2}} \sqrt{b_2}\, \varrho^{\frac{5+\delta}{6}} \left\{ \sqrt{\bar\varrho} + 2 \sqrt[4]{(\varrho+\bar\varrho)\,\bar\varrho} \right\} \\
& - \lambda L^3 c_D \varrho^{\frac{4}{3}} \\
& - \frac{\lambda}{2} L^3 g_6\, b_1^2\, \varrho^2 - \frac{\lambda}{2} c_1 L^3 \varrho^{\frac{1}{3}} \bar\varrho^{\frac{1}{3}} \left(4\varrho + \bar\varrho\right)^{\frac{2}{3}} \\
& + \left\{ \bar\varrho^{\frac{1}{3}} \left(\bar\varrho \varrho^{-1} + 4\right)^{\frac{2}{3}} + \bar\varrho^{\frac{1}{3}} \left(\bar\varrho\varrho^{-1} + 4\right)^{-\frac{1}{3}} + \bar\varrho + 1 + \sigma \right\} O(L^2)\ . 
\end{aligned}
\tag{5.174}
$$

*Proof:* We remark that by Lemmas 5.15 and 5.16 we have

$$
\begin{aligned}
\operatorname{tr}\left( \left| -\triangle - \mu \cdot \mathbf{1} \right| \gamma_{\omega}^{(t)} \right) &\geq \operatorname{tr}\left( \left| -\triangle - \mu \cdot \mathbf{1} \right| p_{\sigma} \right) + \sigma O(L^2) \\
&\geq c_3\, L^3 \varrho^{\frac{5}{3}}\, \sigma^2 + (1+\sigma) O(L^2)\ .
\end{aligned}
\tag{5.175}
$$

The rest follows from Theorem 5.14 and the definition of $R$, given in (5.123). □

We are now ready to minimize over the filling parameter.

**Theorem 5.18.** *Suppose $v = v_{\nu}$, for some $\nu > 0$. Let $\varrho > 0$ be arbitrary and let $\omega$ be an admissible state with the additional property that its two-particle density matrix is trace-class. Then, for sufficiently large density $\varrho > 0$ and sufficiently large size parameter $L$, we have*

$$
\begin{aligned}
& \frac{1}{L^3}\omega(H_{\varrho}) + \frac{2}{5} c_{TF} \varrho^{\frac{5}{3}} + \lambda c_D \varrho^{\frac{4}{3}} + \frac{\lambda}{2} g_6\, b_1^2\, \varrho^2 \\
& \qquad \geq c_3\, \varrho^{\frac{5}{3}} \sigma_*^2 - \lambda \left( c_4(\delta) \varrho^{\frac{8+\delta}{6}} + c_5 \varrho^{\frac{4}{3}} \right) \sqrt[4]{\sigma_*} + \left\{ \sqrt[4]{\sigma_*} + g_6 + 1 \right\} O(L^{-1})\ ,
\end{aligned}
\tag{5.176}
$$

*with*

$$
\sigma_* := \left( \frac{\lambda}{8 c_3} \right)^{\frac{4}{7}} \left( c_4(\delta) \varrho^{\frac{\delta-2}{6}} + c_5 \varrho^{-\frac{1}{3}} + O(L^{-1}) \right)^{\frac{4}{7}}\ , \tag{5.177}
$$

*where we have introduced the constants*

$$
c_4(\delta) = 10\, c_2(\delta)\, g_{\frac{8+\delta}{2}} \sqrt{b_2} \qquad \text{and} \qquad c_5 := 2^{\frac{5}{3}} c_1 = \frac{24}{\pi^2} 7^{\frac{1}{3}} \left(b_1 b_2\right)^{\frac{2}{3}}\ . \tag{5.178}
$$

*Proof:* Let the state $\omega$ comply with the hypothesis of the theorem and set

$$
\bar\varrho := \frac{\operatorname{tr}\left( \gamma_{\omega}^{(t)} \right)}{L^3}\ . \tag{5.179}
$$

We use the estimate given in Theorem 5.17. Note that the relation between $\bar\varrho$ and $\sigma$ given in (5.173) is invertible, and hence the right hand side of (5.174) may be viewed as a function of $\sigma$. We collect all the terms depending on $\sigma$ (without the overall $L^3$ factor)

$$
\begin{aligned}
F(\sigma) \ :=\ & c_3 \varrho^{\frac{5}{3}} \sigma^2 - \lambda c_2(\delta)\, g_{\frac{8+\delta}{2}} \sqrt{b_2}\, \varrho^{\frac{5+\delta}{6}} \left\{ \sqrt{\bar\varrho} + 2 \sqrt[4]{(\varrho+\bar\varrho)\bar\varrho} \right\} \\
& - \lambda \frac{1}{2} c_1 \varrho^{\frac{1}{3}} \bar\varrho^{\frac{1}{3}} \left(4\varrho + \bar\varrho\right)^{\frac{2}{3}} + \left\{ \bar\varrho^{\frac{1}{3}} \left(\bar\varrho\varrho^{-1} + 4\right)^{\frac{2}{3}} + \bar\varrho^{\frac{1}{3}} \left(\bar\varrho\varrho^{-1} + 4\right)^{-\frac{1}{3}} + \sigma + \bar\varrho + 1 \right\} O(L^{-1})\ ,
\end{aligned}
\tag{5.180}
$$

for all $\sigma \in \mathbb{R}_0^+$. (Note that this does not define $F$ as a function, due to the presence of the $O(L^{-1})$ term. $F$ is rather an equivalence class of functions. The following considerations are valid for any function in this class, see also Remark 5.7.)

Corresponding to (5.173), we distinguish two cases.

Case $\bar{\varrho} \geq 4\varrho$:

Note that in this case we have

$$\bar{\varrho} = 4\varrho \left(\frac{1+\sigma}{2}\right)^{\frac{3}{2}} = 4\varrho\tilde{\sigma} \ . \tag{5.181}$$

It is easily seen that

$$\sigma \geq 1 \qquad \text{and} \qquad \tilde{\sigma} := \left(\frac{1+\sigma}{2}\right)^{\frac{3}{2}} \geq 1 \ . \tag{5.182}$$

The parameter $\tilde{\sigma}$ is introduced for notational convenience. We can now estimate

$$\begin{aligned}
F(\sigma) \;&=\; c_3\varrho^{\frac{5}{3}}\sigma^2 - 2\lambda c_2(\delta)\, g_{\frac{8+\delta}{2}}\sqrt{b_2}\,\varrho^{\frac{8+\delta}{6}}\left\{\sqrt{\tilde{\sigma}} + 2\sqrt[4]{\left(\tfrac{1}{4}+\tilde{\sigma}\right)\tilde{\sigma}}\right\} \\
&\quad - 2\lambda c_1\varrho^{\frac{4}{3}}\tilde{\sigma}^{\frac{1}{3}}\,(1+\tilde{\sigma})^{\frac{2}{3}} + \left\{\tilde{\sigma}^{\frac{1}{3}}\,(\tilde{\sigma}+1)^{\frac{2}{3}} + \tilde{\sigma}^{\frac{1}{3}}\,(\tilde{\sigma}+1)^{-\frac{1}{3}} + \tilde{\sigma}+1\right\} O(L^{-1}) \\
&\geq\; c_3\varrho^{\frac{5}{3}}\sigma^2 - 2\lambda c_2(\delta)\, g_{\frac{8+\delta}{2}}\sqrt{b_2}\,\varrho^{\frac{8+\delta}{6}}\left\{1 + 2\sqrt[4]{\tfrac{5}{4}}\right\}\tilde{\sigma} \\
&\quad - 2^{\frac{5}{3}}\lambda c_1\varrho^{\frac{4}{3}}\tilde{\sigma} + (\tilde{\sigma}+1)\,O(L^{-1}) \\
&\geq\; c_3\varrho^{\frac{5}{3}}\sigma^2 - \lambda c_4(\delta)\varrho^{\frac{8+\delta}{6}}\left(\frac{1+\sigma}{2}\right)^{\frac{3}{2}} \\
&\quad - \lambda c_5\varrho^{\frac{4}{3}}\left(\frac{1+\sigma}{2}\right)^{\frac{3}{2}} + \left(\frac{1+\sigma}{2}\right)^{\frac{3}{2}} O(L^{-1}) + O(L^{-1}) \\
&=: H_1(\sigma) \ .
\end{aligned} \tag{5.183}$$

We have introduced the constants

$$c_4(\delta) = 10\, c_2(\delta) g_{\frac{8+\delta}{2}}\sqrt{b_2} \qquad \text{and} \qquad c_5 := 2^{\frac{5}{3}}c_1 \ . \tag{5.184}$$

We estimated

$$1 + 2\sqrt[4]{\tfrac{5}{4}} \;\leq\; 5 \ . \tag{5.185}$$

By taking the derivative of $H_1$ with respect to $\sigma$, it is easily seen that $H_1$ is monotone nondecreasing in $[1,\infty)$, if $\varrho$ and $L$ are sufficiently large. In this case, we thus conclude that

$$F(\sigma) \;\geq\; H_1(1) \;=\; c_3\varrho^{\frac{5}{3}} - \lambda c_4(\delta)\varrho^{\frac{8+\delta}{6}} - \lambda c_5\varrho^{\frac{4}{3}} + O(L^{-1}) \quad , \qquad \forall\, \sigma \geq 1 \ , \tag{5.186}$$

for sufficiently large density $\varrho$ and sufficiently large size parameter $L$.

Case $\bar{\varrho} < 4\varrho$: Note that in this case we have

$$\bar{\varrho} = 4\varrho\sigma \qquad \text{and} \qquad \sigma < 1 \ . \tag{5.187}$$

We can now estimate (similarly to (5.183))

$$\begin{aligned}
F(\sigma) \ &= \ c_3\varrho^{\frac{5}{3}}\sigma^2 - 2\lambda c_2(\delta)\, g_{\frac{8+\delta}{2}}\sqrt{b_2}\,\varrho^{\frac{8+\delta}{6}}\left\{\sqrt{\sigma} + 2\sqrt[4]{\left(\tfrac{1}{4}+\sigma\right)\sigma}\right\} \\
&\quad - 2\lambda c_1\varrho^{\frac{4}{3}}\sigma^{\frac{1}{3}}\left(1+\sigma\right)^{\frac{2}{3}} + \left\{\sigma^{\frac{1}{3}}\left(\sigma+1\right)^{\frac{2}{3}} + \sigma^{\frac{1}{3}}\left(\sigma+1\right)^{-\frac{1}{3}} + \sigma + 1\right\} O(L^{-1}) \\
&\geq \ c_3\varrho^{\frac{5}{3}}\sigma^2 - 2\lambda c_2(\delta)\, g_{\frac{8+\delta}{2}}\sqrt{b_2}\varrho^{\frac{8+\delta}{6}}\left\{1 + 2\sqrt[4]{\tfrac{5}{4}}\right\}\sqrt[4]{\sigma} \\
&\quad - \lambda 2^{\frac{5}{3}}c_1\varrho^{\frac{4}{3}}\sqrt[4]{\sigma} + \left(\sigma^{\frac{1}{4}}+1\right) O(L^{-1}) \\
&\geq \ c_3\varrho^{\frac{5}{3}}\sigma^2 - \lambda\, c_4(\delta)\,\varrho^{\frac{8+\delta}{6}}\sqrt[4]{\sigma} - \lambda c_5\varrho^{\frac{4}{3}}\sqrt[4]{\sigma} + \left(\sqrt[4]{\sigma}+1\right) O(L^{-1}) \\
&=: H_2(\sigma) \ .
\end{aligned} \tag{5.188}$$

By taking the derivative of $H_2$, seen as a function on $\mathbb{R}^+$, and equating it to zero, we deduce that $H_2$ has a unique global minimum at

$$\sigma_* := \left(\frac{\lambda}{8c_3}\right)^{\frac{4}{7}}\left(c_4(\delta)\varrho^{\frac{\delta-2}{6}} + c_5\varrho^{-\frac{1}{3}} + O(L^{-1})\right)^{\frac{4}{7}} \ . \tag{5.189}$$

Remember that $\delta \in [0,1]$ and note that for sufficiently large $\varrho$ and sufficiently large size parameter $L$, we have

$$\sigma_* \in [0,1] \ . \tag{5.190}$$

Thus we have

$$F(\sigma) \geq H_2(\sigma_*) \quad , \qquad \forall\, \sigma \in [0,1] \ , \tag{5.191}$$

for sufficiently large size parameter $L$ and sufficiently large density $\varrho$.

The claim of the theorem follows from (5.186), (5.191) and from the observation

$$H_1(1) = H_2(1) \geq H_2(\sigma_*) \ . \tag{5.192}$$

□

**Thermodynamic Limit**

The ground state energy density $e_0$ of the Fermionic Jellium Model (in the thermodynamic limit) is defined to be

$$e_0 := \lim_{L\to\infty}\frac{1}{L^3}\inf\left\{\ \omega\left(H_\varrho\right) - E_{bb}\ \middle|\ \omega \text{ admissible, with } M_\omega \text{ trace-class}\ \right\} \ , \tag{5.193}$$

where the quantity $E_{bb}$ is given by

$$E_{bb} := \frac{1}{2}\varrho J_\varrho = \frac{\lambda}{2}\varrho^2 b_1^2 g_6 \ . \tag{5.194}$$

It is interpreted as the background self-energy. We recall that $M_\omega$ denotes the two-particle density matrix of the state $\omega$. The constants $b_1$ and $g_6$ are given in (5.79).

**Theorem 5.19.** *Suppose $v = v_\nu$, for some $\nu > 0$ and let $\lambda > 0$ be given. Then the ground state energy density of the Fermionic Jellium Model in the thermodynamic limit $e_0$, defined in* (5.193)*, has the following behavior for large densities $\varrho$:*

$$e_0 \geq -\frac{2}{5} c_{TF} \varrho^{\frac{5}{3}} - \lambda c_D \varrho^{\frac{4}{3}} + \varrho^{\frac{4}{3}} O(\varrho^{\frac{4\delta-1}{21}}) \ , \tag{5.195}$$

*for any $\delta \in (0,1)$. $c_{TF}$ and $c_D$ denote the Thomas-Fermi constant and Dirac's constant, respectively. They are given in* (5.99) *and* (5.116).

*Proof:* From Theorem 5.18 we obtain, for sufficiently large density $\varrho$, that

$$e_0 + \frac{2}{5} c_{TF} \varrho^{\frac{5}{3}} + \lambda c_D \varrho^{\frac{4}{3}} \geq c_3 \varrho^{\frac{5}{3}} \tilde{\sigma}_*^2 - \lambda \left( c_4(\delta) \varrho^{\frac{8+\delta}{6}} + c_5 \varrho^{\frac{4}{3}} \right) \sqrt[4]{\tilde{\sigma}_*} \ , \tag{5.196}$$

with

$$\tilde{\sigma}_* := \left( \frac{\lambda}{8c_3} \right)^{\frac{4}{7}} \left( c_4(\delta) \varrho^{\frac{\delta-2}{6}} + c_5 \varrho^{-\frac{1}{3}} \right)^{\frac{4}{7}} \ . \tag{5.197}$$

By Taylor's Theorem, we have[2]

$$\tilde{\sigma}_* = \left( \frac{\lambda c_4(\delta)}{8c_3} \right)^{\frac{4}{7}} \varrho^{\frac{2\delta-4}{21}} + o\left( \varrho^{-\frac{\delta+4}{21}} \right) \ , \qquad (\varrho \longrightarrow \infty) \ .$$

Using again Taylor's Theorem, this leads to the asymptotic behavior of the following expressions involving $\tilde{\sigma}_*$ and $\varrho$:

$$\begin{aligned}
\varrho^{\frac{5}{3}} (\tilde{\sigma}_*)^2 &= \left( \frac{\lambda c_4(\delta)}{8c_3} \right)^{\frac{8}{7}} \varrho^{\frac{4\delta+27}{21}} + o\left( \varrho^{\frac{\delta+27}{21}} \right) \ , && (\varrho \longrightarrow \infty) \ , \\
\varrho^{\frac{8+\delta}{6}} (\tilde{\sigma}_*)^{\frac{1}{4}} &= \left( \frac{\lambda c_4(\delta)}{8c_3} \right)^{\frac{1}{7}} \varrho^{\frac{4\delta+27}{21}} + o\left( \varrho^{\frac{\delta+27}{21}} \right) \ , && (\varrho \longrightarrow \infty) \ , \\
\varrho^{\frac{4}{3}} (\tilde{\sigma}_*)^{\frac{1}{4}} &= \left( \frac{\lambda c_4(\delta)}{8c_3} \right)^{\frac{1}{7}} \varrho^{\frac{\delta+54}{42}} + o\left( \varrho^{\frac{-5\delta+54}{42}} \right) \ , && (\varrho \longrightarrow \infty) \ .
\end{aligned}$$

These terms correspond to the three terms on the right hand side of (5.196). Obviously, the first two of these three terms dominate the behavior for large $\varrho$. Therefore, we obtain from (5.196)

$$\begin{aligned}
e_0 + \frac{2}{5} c_{TF} \varrho^{\frac{5}{3}} + \lambda c_D \varrho^{\frac{4}{3}} &\geq \left( \frac{\lambda c_4(\delta)}{8c_3} \right)^{\frac{8}{7}} \varrho^{\frac{4\delta+27}{21}} + o\left( \varrho^{\frac{\delta+27}{21}} \right) \\
&= O\left( \varrho^{\frac{4\delta+27}{21}} \right) = \varrho^{\frac{4}{3}} O(\varrho^{\frac{4\delta-1}{21}}) \ .
\end{aligned} \tag{5.199}$$

The proof is complete. □

We remark that for $v = v_\nu$, we have $b_1 = \pi^{\frac{3}{2}}$ and $g_6 = \frac{4}{\pi^2} \frac{1}{\nu^2}$.

[2] Actually, we have the slightly better behavior:

$$\tilde{\sigma}_* = \left( \frac{\lambda c_4(\delta)}{8c_3} \right)^{\frac{4}{7}} \varrho^{\frac{2\delta-4}{21}} + O\left( \varrho^{-\frac{3\delta+8}{42}} \right) \ , \qquad (\varrho \longrightarrow \infty) \ . \tag{5.198}$$

## 5.2 Bosonic Theory

### 5.2.1 A Bosonic Wick Theorem

In this subsection we prove a generalization of a combinatorial identity known as Wick Theorem. We freely write down polynomials in the boson creation and annihilation operators, without worrying about domain questions. All the relations we write down are valid on the domain of finite vectors or, more importantly, as equalities in expectation values of analytic states. The latter case is the case we are actually interested in.

**Definition 5.20.** *Denote by $a(\cdot)$ and $a^*(\cdot)$ the generators of the CCR Algebra. We then associate to any monomial*

$$a^{\tau_1}(f_1)\cdots a^{\tau_n}(f_n) \quad , \qquad \forall\, n \in \mathbb{N},\ \tau_1,\ldots,\tau_n \in \{\varnothing, *\},\ f_1,\ldots,f_n \in \mathcal{H}^1 \ , \tag{5.200}$$

*a monomial, <u>normal-ordered</u> with respect to the Fock representation, by defining*

$$:a^{\tau_1}(f_1)\cdots a^{\tau_n}(f_n): \ := \ a^{\tau_{\pi(1)}}(f_{\pi(1)})\cdots a^{\tau_{\pi(n)}}(f_{\pi(n)}) \ . \tag{5.201}$$

*The permutation $\pi$ is uniquely determined by the conditions*

$$\tau_{\pi(1)} = \cdots = \tau_{\pi(k)} = * \quad , \quad \tau_{\pi(k+1)} = \cdots = \tau_{\pi(n)} = \varnothing \ , \tag{5.202}$$

*for some $k \in \{0,\ldots,n\}$, and*

$$\pi(1) < \cdots < \pi(k) \quad , \quad \pi(k+1) < \cdots < \pi(n) \ . \tag{5.203}$$

*By demanding linearity and setting $:\mathbf{1}: := \mathbf{1}$, we extend this definition to all polynomials in the boson annihilation and creation operators and the identity.*

Note that the elements of the CCR Algebra are equivalence classes of polynomials in the generators $a^*(\cdot)$ and $a(\cdot)$. The normal-ordering is defined on these polynomials, but it is *not* well-defined on the CCR Algebra. We discuss these concepts in more detail in Section B.2.

For any polynomial expression $q$ of degree two in the boson annihilation and creation operators, we define the contraction $[\![\, q \,]\!]$ by:

$$[\![\, q \,]\!] \ := \ q - :q: \ . \tag{5.204}$$

Note that, for all $f_1, f_2 \in \mathcal{H}^1$ and all $\sigma_1, \sigma_2 \in \{\varnothing, *\}$, the following equality holds

$$[\![\, a^{\sigma_1}(f_1)a^{\sigma_2}(f_2) \,]\!] = \begin{cases} 0 & \text{if } a^{\sigma_1}(f_1)a^{\sigma_2}(f_2) \text{ is normal-ordered} \\ [a^{\sigma_1}(f_1), a^{\sigma_2}(f_2)] & \text{else} \end{cases} \ . \tag{5.205}$$

In order to formulate the bosonic Wick Theorem, we introduce, for any $n \in \mathbb{N}$, the set $\mathcal{P}_2(n)$ as follows: $P$ is an element of $\mathcal{P}_2(n)$ if and only if

$$P = \left\{ p^{(1)}, \ldots, p^{(k)} \right\} \ , \tag{5.206}$$

for some $k \in \mathbb{N}_0$ and some pairwise disjoint sets $p^{(1)}, \ldots, p^{(k)}$ of cardinality two, such that

$$p^{(1)},\ \ldots,\ p^{(k)} \ \subseteq \ \{1,\ldots,n\} \ . \tag{5.207}$$

Note that $\varnothing \in \mathcal{P}_2(n)$, for all $n \in \mathbb{N}$ (corresponding to the case $k = 0$).

**Theorem 5.21 (Wick).** *For any $f_1, \ldots, f_n \in \mathcal{H}^1$, all $\sigma_1, \ldots, \sigma_n \in \{\varnothing, *\}$ and arbitrary constants $z_1, \ldots, z_n \in \mathbb{C}$, we abbreviate*

$$a_j := a^{\sigma_j}(f_j) + z_j \quad , \qquad \forall\, j \in \{1, \ldots, n\} \ . \tag{5.208}$$

*It then holds true that*

$$a_1 \cdots a_n = \sum_{P \in \mathcal{P}_2(n)} \left( \prod_{p \in P} [\![\, a_{p_1} a_{p_2} \,]\!] \right) \left( : \prod_{j \in \{1,\ldots,n\} \setminus \bigcup_{p \in P} p} a_j : \right) \ . \tag{5.209}$$

*Proof:* As a first step, we show that

$$:a_1 \cdots a_n: \ = \ :a_1 \cdots a_{n-1}: a_n \ - \ \sum_{l=1}^{n-1} :a_1 \cdots \widehat{a_l} \cdots a_{n-1}: [\![\, a_l a_n \,]\!] \ , \tag{5.210}$$

where the notation $\widehat{a_l}$ indicates that the corresponding factor is omitted from the above product. To show (5.210), let the permutation $\pi \in S_n$ be determined by

$$:a_1 \cdots a_n: \ = \ a_{\pi(1)} \cdots a_{\pi(n)} \tag{5.211}$$

and let $m \in \{1, \ldots, n\}$ be such that $\pi(m) = n$. Then we have:

$$\begin{aligned} :a_1 \cdots a_n: &= a_{\pi(1)} \cdots a_{\pi(m)} \cdots a_{\pi(n)} \\ &= a_{\pi(1)} \cdots \widehat{a_{\pi(m)}} \cdots a_{\pi(n)} a_n + \sum_{l=m+1}^{n} a_{\pi(1)} \cdots \widehat{a_{\pi(m)}} \cdots \widehat{a_{\pi(l)}} \cdots a_{\pi(n)} \left[ a_n, a_{\pi(l)} \right] \ . \end{aligned} \tag{5.212}$$

Note that all the commutators appearing on the very right of this relation, are of one of the following three types:

$$\left[ a^*(f_{\pi(m)}) + z_n, a^*(f_{\pi(l)}) + z_{\pi(l)} \right] \ , \tag{5.213a}$$

$$\left[ a^*(f_{\pi(m)}) + z_n, a(f_{\pi(l)}) + z_{\pi(l)} \right] \ , \tag{5.213b}$$

$$\left[ a(f_{\pi(m)}) + z_n, a(f_{\pi(l)}) + z_{\pi(l)} \right] \ . \tag{5.213c}$$

Therefore, by relation (5.205), we have

$$[\![\, a_{\pi(l)} a_{\pi(m)} \,]\!] = - \left[ a_{\pi(m)}, a_{\pi(l)} \right] \quad , \qquad \forall\, l \in \{m+1, \ldots, n\} \ .$$

Furthermore, we have for $l < m$

$$[\![\, a_{\pi(l)} a_{\pi(m)} \,]\!] = 0 \quad , \qquad \forall\, l \in \{1, \ldots, m-1\} \ .$$

Thus it follows

$$\begin{aligned} :a_1 \cdots a_n: &= a_{\pi(1)} \cdots \widehat{a_{\pi(m)}} \cdots a_{\pi(n)} a_n - \sum_{l \in M_n \setminus \{m\}} a_{\pi(1)} \cdots \widehat{a_{\pi(m)}} \cdots \widehat{a_{\pi(l)}} \cdots a_{\pi(n)} [\![\, a_{\pi(l)} a_n \,]\!] \\ &= :a_1 \cdots a_{n-1}: a_n - \sum_{l=1}^{n-1} :a_1 \cdots \widehat{a_l} \cdots a_{n-1}: [\![\, a_l a_n \,]\!] \ , \end{aligned} \tag{5.214}$$

where we have defined

$$M_n := \{1, \ldots, n\} \quad , \qquad \forall\, n \in \mathbb{N}\ . \tag{5.215}$$

This proves (5.210). We proceed to prove (5.209) by an induction argument. First note that the claim of the theorem is trivial for $n = 1$. Secondly, let a $n \in \mathbb{N}$ be given and assume (5.209) was true for this $n$. We then prove

$$a_1 \cdots a_{n+1} = \sum_{P \in \mathcal{P}_2(n+1)} \left( \prod_{p \in P} [\![\, a_{p_1} a_{p_2} \,]\!] \right) \left( :\prod_{j \in M_{n+1} \setminus \bigcup_{p \in P} p} a_j : \right) . \tag{5.216}$$

For the right hand side (r. h. s) of (5.216), we have

$$\begin{aligned}
\text{r. h. s.} &= \sum_{P \in \mathcal{P}_2(n+1)} \left( \prod_{p \in P} [\![\, a_{p_1} a_{p_2} \,]\!] \right) \left( :\prod_{j \in M_{n+1} \setminus \bigcup_{p \in P} p} a_j : \right) \\
&= \sum_{P \in \mathcal{P}_2(n)} \left( \prod_{p \in P} [\![\, a_{p_1} a_{p_2} \,]\!] \right) \left( :\prod_{j \in M_{n+1} \setminus \bigcup_{p \in P} p} a_j : \right) \\
&\quad + \sum_{P \in \mathcal{P}_2(n)} \sum_{l \in M_n \setminus \bigcup_{p \in P} p} [\![\, a_l a_{n+1} \,]\!] \left( \prod_{p \in P} [\![\, a_{p_1} a_{p_2} \,]\!] \right) \left( :\prod_{j \in M_n \setminus \left( \bigcup_{p \in P} p\, \cup\, \{l\} \right)} a_j : \right) .
\end{aligned} \tag{5.217}$$

Here, we decompose the sum over all $P \in \mathcal{P}_2(n+1)$ into the sum over all $P \in \mathcal{P}_2(n)$ and the sum over all

$$P \ \in\ \mathcal{P}_2(n+1) \setminus \mathcal{P}_2(n) \ =\ \bigcup_{P \in \mathcal{P}_2(n)} \ \bigcup_{l \in M_n \setminus \bigcup_{p \in P} p} P \cup \{l, n+1\}\ . \tag{5.218}$$

By relation (5.210) we have

$$\begin{aligned}
:\prod_{j \in M_{n+1} \setminus \bigcup_{p \in P} p} a_j : \ &= \left( :\prod_{j \in M_n \setminus \bigcup_{p \in P} p} a_j : \right) a_{n+1} \\
&\quad - \sum_{l \in M_n \setminus \bigcup_{p \in P} p} [\![\, a_l a_{n+1} \,]\!] \left( :\prod_{j \in M_n \setminus \left( \bigcup_{p \in P} p\, \cup\, \{l\} \right)} a_j : \right) \quad ,
\end{aligned} \tag{5.219}$$

for all $P \in \mathcal{P}_2(n)$. Note that inserting this relation into (5.217) leads to a cancellation. Thus, we obtain

$$\text{r. h. s.} = \left( \sum_{P \in \mathcal{P}_2(n)} \left( \prod_{p \in P} [\![\, a_{p_1} a_{p_2} \,]\!] \right) \left( :\prod_{j \in n \setminus \bigcup_{p \in P} p} a_j : \right) \right) a_{n+1}\ . \tag{5.220}$$

This is equal to the left hand side of (5.216) by the induction hypothesis. $\square$

An important consequence of relation (5.205) is that the contractions of any homogeneously quadratic expression in the boson annihilation and creation operators, may be expressed as a vacuum expectation value, i .e.,

$$[\![\, B(f) B(g) \,]\!] = \Omega\big( B(f) B(g) \big) \quad , \qquad \forall\, f, g \in \mathcal{K}\ . \tag{5.221}$$

Any linear expression and any scalar has vanishing contraction. Therefore, we may rewrite the contractions appearing in the Wick Theorem in terms of vacuum expectation values.

For any Bogoliubov transformation $(w, v)$, denoting by $\alpha_{(w,v)}$ the associated algebra automorphism, we introduce the normal-ordering with respect to $(w, v)$, as follows:

$$: \cdot :_{(w,v)} \ := \ \alpha^{-1}_{(w,v)} \left( :\alpha_{(w,v)} ( \ \cdot \ ) : \right) \ . \tag{5.222}$$

We generalize the Wick Theorem to the normal-ordering $: \cdot :_{(w,v)}$.

**Corollary 5.22.** *Let $(w, v)$ be a Bogoliubov transformation and let $f_1, \ldots, f_n \in \mathcal{K}$ be arbitrary. Denote the generators $B(f_1), \ldots, B(f_n)$ of the bosonic self-dual algebra by $B_1, \ldots, B_n$ and denote by $v_1, \ldots, v_n$ the scalars $v(f_1), \ldots, v(f_n)$. It then holds*

$$B_1 \cdots B_n = \sum_{P \in \mathcal{P}_2(n)} \left( \prod_{p \in P} \left( \Omega_{(w,v)} \left( B_{p_1} B_{p_2} \right) - v_{p_1} v_{p_2} \right) \right) \left( : \prod_{j \in \{1,\ldots,n\} \setminus \bigcup_{p \in P} p} B_j :_{(w,v)} \right) , \tag{5.223}$$

*where we have denoted*

$$\Omega_{(w,v)}(\cdot) \ := \ \Omega\big( \alpha_{(w,v)}(\cdot) \big) \ . \tag{5.224}$$

*Proof:* We remark that the transformed generators are of the form

$$\alpha_{(w,v)}\big(B(f_j)\big) = B(wf_j) + v(f_j) \quad , \qquad \forall \ j \in \{1, \ldots, n\} \ . \tag{5.225}$$

By Theorem 5.21 we may write:

$$\begin{aligned} \alpha_{(w,v)}(B_1 \cdots B_n) = \sum_{P \in \mathcal{P}_2(n)} & \left( \prod_{p \in P} \left[\!\left[ \ \big(B(wf_{p_1}) + v(f_{p_1})\big)\big(B(wf_{p_2}) + v(f_{p_2})\big) \ \right]\!\right] \right) \\ & \cdot \left( : \prod_{j \in M_n \setminus \bigcup_{p \in P} p} \big(B(wf_j) + v(f_j)\big) : \right) , \end{aligned} \tag{5.226}$$

where we have used notation (5.215). Due to (5.221) and the fact that expressions linear in the generators of the CCR Algebra and scalars have vanishing contractions, we have

$$\begin{aligned} & \alpha_{(w,v)}(B_1 \cdots B_n) = \\ & = \sum_{P \in \mathcal{P}_2(n)} \left( \prod_{p \in P} \Omega\big(B(wf_{p_1}) B(wf_{p_2})\big) \right) \left( : \prod_{j \in M_n \setminus \bigcup_{p \in P} p} \big(B(wf_j) + v(f_j)\big) : \right) \ . \end{aligned} \tag{5.227}$$

From this statement we arrive at the claim, by taking the Bogoliubov transformation $\alpha^{-1}_{(w,v)}$ of both sides and by remembering that

$$\Omega_{(w,v)}\big(B(f)B(g)\big) = \Omega\big(B(wf)B(wg)\big) + v(f)v(g) \ . \tag{5.228}$$

□

In the case $n = 4$, we can rewrite the claim of Corollary 5.22, as follows.

$$
\begin{aligned}
B_1 \cdots B_4 &= \\
&= \sum_{\pi \text{ Pairing}} \Big\{ :B_{\pi(1)} B_{\pi(2)}:_{(w,v)} \big( \Omega_{(w,v)}(B_{\pi(3)} B_{\pi(4)}) - v_{\pi(3)} v_{\pi(4)} \big) \\
&\qquad + :B_{\pi(3)} B_{\pi(4)}:_{(w,v)} \big( \Omega_{(w,v)}(B_{\pi(1)} B_{\pi(2)}) - v_{\pi(1)} v_{\pi(2)} \big) \\
&\qquad + \big( \Omega_{(w,v)}(B_{\pi(1)} B_{\pi(2)}) - v_{\pi(1)} v_{\pi(2)} \big) \big( \Omega_{(w,v)}(B_{\pi(3)} B_{\pi(4)}) - v_{\pi(3)} v_{\pi(4)} \big) \Big\} ,
\end{aligned} \tag{5.229}
$$

where the sums extend over all pairings, i. e., over all

$$
\pi \in S_4 , \qquad \text{with} \qquad 1 = \pi(1) < \pi(3) \quad , \quad \pi(2) < \pi(4) . \tag{5.230}
$$

Observing that

$$
:B(f)B(g):_{(w,v)} = B(f)B(g) - \Big( \Omega_{(w,v)}\big(B(f)B(g)\big) - v(f)v(g) \Big) , \tag{5.231}
$$

for all $f, g \in \mathcal{K}$, we obtain:

**Corollary 5.23.** *Under the hypothesis of Corollary 5.22, we have:*

$$
\begin{aligned}
B_1 \cdots B_4 \ &= \ :B_1 \cdots B_4:_{(w,v)} \\
&+ \sum_{\pi \text{ Pairing}} \Big\{ B_{\pi(1)} B_{\pi(2)} \big( \Omega_{(w,v)}(B_{\pi(3)} B_{\pi(4)}) - v_{\pi(3)} v_{\pi(4)} \big) \\
&\qquad + B_{\pi(3)} B_{\pi(4)} \big( \Omega_{(w,v)}(B_{\pi(1)} B_{\pi(2)}) - v_{\pi(1)} v_{\pi(2)} \big) \Big\} \\
&- \sum_{\pi \text{ Pairing}} \big( \Omega_{(w,v)}(B_{\pi(1)} B_{\pi(2)}) - v_{\pi(1)} v_{\pi(2)} \big) \big( \Omega_{(w,v)}(B_{\pi(3)} B_{\pi(4)}) - v_{\pi(3)} v_{\pi(4)} \big) ,
\end{aligned} \tag{5.232}
$$

*where the sum extends over all $\pi$ obeying* (5.230)*.*

### 5.2.2 Derivation of a Correlation Estimate

In this subsection we give a lower bound on the expectation values of quartic polynomials in the boson creation and annihilation operators of the following type

$$
\sum_{p,q \in \mathbb{N}} :a^*(Df_p) a^*(Df_q) a(Df_q) a(Df_p):_{(w,v)} . \tag{5.233}
$$

Here, we have fixed an orthonormal basis $\{f_j\}_{j \in \mathbb{N}}$ in $\mathcal{H}^1$ and denoted by $D$ some nonnegative operator in $\mathcal{B}(\mathcal{H}^1)$. The pair $(w, v)$ denotes a bosonic Bogoliubov transformation. The following derivation parallels the derivation of the fermionic correlation estimate in Subsection 5.1.2. We hope that some day it will be useful to estimate the ground state energy of the Bosonic Jellium Model, possibly simplifying the sofisticated arguments given by Lieb and Solovej in [23, 24]. Some of the following arguments appear already in [7].

In order to formulate the main theorem of this subsection, let $(w, v)$ be a Bogoliubov transformation of the form

$$
w = \begin{pmatrix} X & Y \\ \bar{Y} & \bar{X} \end{pmatrix} , \qquad \text{for some} \qquad X, Y \in \mathcal{B}(\mathcal{H}^1) , \tag{5.234}
$$

and

$$v\left(\left(\begin{array}{c} f^+ \\ f^- \end{array}\right)\right) = \langle u \,|\, f^+ \rangle + \langle \bar{u} \,|\, f^- \rangle \ , \qquad \text{for some} \qquad u \in \mathcal{H}^1 \ . \tag{5.235}$$

Suppose furthermore that $(w, v)$ possesses a unitary implementation $U$ in $\mathcal{F}_+$.

**Theorem 5.24.** *Let $\omega$ be an arbitrary admissible state with the additional property that*

$$\tilde{\omega}\big(\,\mathbf{n}^2\,\big) := \sum_{p,q \in \mathbb{N}} \tilde{\omega}\big(a^*(f_p)a(f_p)a^*(f_q)a(f_q)\big) < \infty \ , \tag{5.236}$$

*where $\tilde{\omega}$ denotes the state given by*

$$\tilde{\omega}(\cdot) := \omega(U^* \ \cdot \ U) \ . \tag{5.237}$$

*Denote furthermore by $\delta_\omega \in \mathcal{H}^1$ the vector determined by*

$$\langle \delta_\omega \,|\, f \rangle = \omega\big(a^*(f)\big) \quad , \qquad \forall \ f \in \mathcal{H}^1 \ . \tag{5.238}$$

*Setting*

$$\tilde{\delta} := X\delta_\omega - Y\bar{\delta}_\omega + Y\bar{u} - Xu \ , \tag{5.239}$$

$$\begin{aligned} \tilde{\gamma} := {} & X\gamma_\omega X^* - Y\alpha_\omega^* X^* - X\alpha_\omega Y^* + Y(1+\bar{\gamma}_\omega)Y^* \\ & - \big|\, Xu - Y\bar{u}\rangle \, \langle X\delta - Y\bar{\delta}\,\big| - \big|\, X\delta - Y\bar{\delta}\rangle \, \langle Xu - Y\bar{u}\,\big| \\ & + |\, Xu - Y\bar{u}\rangle \, \langle Xu - Y\bar{u}\,| \ , \end{aligned} \tag{5.240}$$

*where $X$, $Y$ and $u$ are given in* (5.234) *and* (5.235)*, respectively. Then we have the following correlation estimate:*

$$\begin{aligned} & \sum_{p,q \in \mathbb{N}} \omega\Big(:a^*(Df_p)a^*(Df_q)a(Df_q)a(Df_p):_{(w,v)}\Big) \\ & \geq -2^{\frac{5}{2}} \operatorname{tr}\big(\bar{D}^2 Y^* Y\big) \Big\{ \operatorname{tr}\big(\bar{D}^2 Y^* Y\big)\, \tilde{\omega}\left(\mathbf{n}^2\right) + \operatorname{tr}\big(\bar{D}^2 Y^* \gamma Y\big) \Big\}^{\frac{1}{2}} \Big\{ \|\, XD^2X^* \,\|\, \tilde{\omega}\left(\mathbf{n}^2\right) \\ & \qquad + \tilde{\omega}(\mathbf{n})\,\|\, Du \,\|^2 \Big\}^{\frac{1}{2}} \\ & \quad -4 \operatorname{tr}\big(\bar{D}^2 Y^* Y\big) \Big[ \operatorname{tr}\big(D^2X^*\tilde{\gamma}X\big) + 2\operatorname{Re}\Big\langle \tilde{\delta} \,\big|\, XD^2u \Big\rangle + \|\, Du \,\|^2 \\ & \qquad + \|\, XD^2X^* \,\|\, \tilde{\omega}\left(\mathbf{n}^2\right) + \tilde{\omega}(\mathbf{n})\,\|\, Du \,\|^2 \Big] \\ & \quad -2 \Big\{ \operatorname{tr}\big(\bar{D}^2 Y^* Y\big) \Big[ 2\operatorname{Re}\Big\langle \tilde{\delta} \,\big|\, XD^2u \Big\rangle + \|\, Du \,\|^2 + 2\operatorname{tr}\big(D^2X^*\tilde{\gamma}X\big) + 2\tilde{\omega}(\mathbf{n})\,\|\, Du \,\|^2 \\ & \qquad + 2\,\|\, XD^2X^* \,\|\, \tilde{\omega}\left(\mathbf{n}^2\right) \Big] + 2\,\Big|\Big\langle u \,\Big|\, D^2Y^T\bar{Y}D^2X^*\tilde{\delta} \Big\rangle\Big| + \langle u \,|\, D^2Y^T\bar{Y}D^2u \rangle \Big\}^{\frac{1}{2}} \\ & \qquad \cdot \Big\{ 2\,\big|\operatorname{tr}\big(D^2Y^T\bar{X}\bar{D}^2Y^*\tilde{\gamma}X\big)\big| + 2\,\Big|\Big\langle u \,\Big|\, D^2Y^T\bar{X}\bar{D}^2Y^*\tilde{\delta} \Big\rangle\Big| + \operatorname{tr}\big(\bar{D}^2Y^*XD^2Y^T\bar{X}\big) \\ & \qquad + \operatorname{tr}\big(D^2X^*XD^2Y^T(\mathbf{1}+\tilde{\gamma}^T)\bar{Y}\big) + 4\,\Big|\Big\langle u \,\Big|\, D^2Y^T\bar{Y}D^2X^*\tilde{\delta} \Big\rangle\Big| \\ & \qquad + 2\,\langle u \,|\, D^2Y^T\bar{Y}D^2u \rangle + \operatorname{tr}\big(\bar{D}^2Y^*Y\big) \Big[ 2\operatorname{Re}\Big\langle \tilde{\delta} \,\big|\, XD^2u \Big\rangle + \|\, Du \,\|^2 \\ & \qquad\qquad + 3\operatorname{tr}\big(D^2X^*\tilde{\gamma}X\big) + 2\tilde{\omega}(\mathbf{n})\,\|\, Du \,\|^2 + 2\,\|\, XD^2X^* \,\|\, \tilde{\omega}\left(\mathbf{n}^2\right) \Big] \Big\}^{\frac{1}{2}} \ . \end{aligned}$$

Before we proceed to prove this theorem (see p. 132), let us clarify the role of $\tilde{\gamma}$ and $\tilde{\delta}$ with the following lemma.

**Lemma 5.25.** *The state $\tilde{\omega}$ given in* (5.237) *is admissible and its density matrix $\tilde{\gamma}$ is given by* (5.240)*. Furthermore, the vector $\tilde{\delta}$, determined by*

$$\left\langle \tilde{\delta} \,|\, f \right\rangle = \tilde{\omega}\big(a^*(f)\big) \quad , \qquad \forall\ f \in \mathcal{H}^1 \ , \tag{5.241}$$

*is of the form* (5.239)*.*

*Proof:* As we have seen in (2.4), the Bogoliubov transformation inverse to $(w, v)$ is given by

$$\Big(w^{-1}, -v\big(w^{-1}(\cdot)\big)\Big) \qquad \text{with} \qquad w^{-1} = \begin{pmatrix} X^* & -Y^T \\ -Y^* & X^T \end{pmatrix} \ . \tag{5.242}$$

First, we show that $\tilde{\delta}$ is of the form (5.239). We have, for any $f \in \mathcal{H}^1$:

$$\begin{aligned} \left\langle \tilde{\delta} \,|\, f \right\rangle &= \omega\left(a^*(X^* f) - a(Y^T \bar{f}) - \langle u \,|\, X^* f \rangle + \langle \bar{u} \,|\, Y^* f \rangle\right) \\ &= \langle \delta_\omega \,|\, X^* f \rangle - \langle \bar{\delta}_\omega \,|\, Y^* f \rangle - \langle u \,|\, X^* f \rangle + \langle \bar{u} \,|\, Y^* f \rangle \\ &= \left\langle X\delta_\omega - Y\bar{\delta}_\omega - Xu + Y\bar{u} \,|\, f \right\rangle \ . \end{aligned} \tag{5.243}$$

Thus (5.239) follows.

Secondly, we show that $\tilde{\gamma}$ is of the form (5.240). We have, for any $f, g \in \mathcal{H}^1$:

$$\begin{aligned} &\langle f \,|\, \tilde{\gamma} g \rangle = \tilde{\omega}\big(a^*(g) a(f)\big) \\ &\quad = \omega\Big(\big[a^*(X^* g) - a(Y^T \bar{g}) + \langle Y\bar{u} - Xu \,|\, g \rangle\big] \big[a(X^* f) - a^*(Y^T \bar{f}) + \langle f \,|\, Y\bar{u} - Xu \rangle\big]\Big) \ . \end{aligned}$$

Similarly to (5.243), we obtain from this

$$\begin{aligned} \langle f \,|\, \tilde{\gamma} g \rangle = \omega&\Big(\big[a^*(X^* g) - a(Y^T \bar{g})\big] \big[a(X^* f) - a^*(Y^T \bar{f})\big]\Big) \\ &+ \left\langle f \,\middle|\, X\delta - Y\bar{\delta} \right\rangle \langle Y\bar{u} - Xu \,|\, g \rangle + \langle f \,|\, Y\bar{u} - Xu \rangle \left\langle X\delta - Y\bar{\delta} \,|\, g \right\rangle \\ &+ \langle Y\bar{u} - Xu \,|\, g \rangle \langle f \,|\, Y\bar{u} - Xu \rangle \ . \end{aligned} \tag{5.244}$$

The last three terms of this relation correspond to the last three terms in (5.240). As far as the first term, involving the state $\omega$, is concerned, we note that it corresponds to the upper left block of $\Gamma_{\tilde{\omega}}$. Using (5.244) and

$$\Gamma_{\tilde{\omega}} = w \Gamma_\omega w^{-1} \ , \tag{5.245}$$

it easily follows that $\tilde{\gamma}$ is of the form (5.240).

The admissibility of $\tilde{\omega}$ follows from the fact that $\gamma_\omega$ is trace-class and the fact that $\alpha_\omega$ and $Y$ are Hilbert-Schmidt. $\square$

Let us shortly comment on the quality of the above correlation estimate. As is easily seen, we have

$$\omega\Big( \sum_{p,q\in\mathbb{N}} :a_p^* a_q^* a_q a_p:_{(w,v)} \Big) = \| \, Du \, \|^4 \ , \tag{5.246}$$

if $\omega$ and $(w,v)$ are such that $\tilde{\omega} = \Omega$. In this case, the bound in Theorem 5.24 is sharp if and only if we additionally have $u = 0$, i. e., if and only if the Bogoliubov transformation is homogenous. This happens because we have tailored this estimate after the pattern of the fermionic correlation estimate, where we considered exclusively homogenous transformations. It would be desirable to modify the above estimate in such a way, as to ensure that the resulting correlation inequality remains sharp, even for $u \neq 0$. Note furthermore, that according to Corollary 5.23, expression (5.233) cannot be directly interpreted as the approximation error of HFB-Theory.

*Proof of Theorem 5.24:* Let $(w,v)$ be any Bogoliubov transformation obeying (5.234) and (5.235) and let $D$ be an arbitrary nonnegative operator in $\mathcal{B}(\mathcal{H}^1)$. In order to simplify the notation for the purpose of the following, somewhat lengthy calculation, let us abbreviate:

$$a_p^* := a^*(Df_p) \ , \quad c_p^* := a^*(XDf_p) + \langle u \,|\, Df_p \rangle \ , \quad d_p^* := a^*(Y\overline{Df_p}) \ , \tag{5.247}$$

for all $p \in \mathbb{N}$. We then have

$$\omega\Big( \sum_{p,q\in\mathbb{N}} :a_p^* a_q^* a_q a_p:_{(w,v)} \Big) = \sum_{p,q\in\mathbb{N}} \tilde{\omega}\left( :(c_p + d_p^*)^*(c_q + d_q^*)^*(c_q + d_q^*)(c_p + d_p^*): \right) \ . \tag{5.248}$$

Note that the normal-ordering applies to the $c$'s and $d$'s in just the same way as it does to the $a$'s: Generators bearing a $*$ are moved to the left, neglecting any commutators.

We have

$$\begin{aligned} \tilde{\omega}\Big( \sum_{p,q\in\mathbb{N}} :a_p^* a_q^* a_q a_p: \Big) = \sum_{p,q\in\mathbb{N}} \Big\{ & \tilde{\omega}\big(:c_p^* c_q^* c_q c_p:\big) + \tilde{\omega}\big(:c_p^* c_q^* c_q d_p^*:\big) + \tilde{\omega}\big(:c_p^* c_q^* d_q^* c_p:\big) \\ & + \tilde{\omega}\big(:c_p^* d_q c_q c_p:\big) + \tilde{\omega}\big(:d_p c_q^* c_q c_p:\big) + \tilde{\omega}\big(:c_p^* c_q^* d_q^* d_p^*:\big) \\ & + \tilde{\omega}\big(:c_p^* d_q c_q d_p^*:\big) + \tilde{\omega}\big(:c_p^* d_q d_q^* c_p:\big) + \tilde{\omega}\big(:d_p c_q^* c_q d_p^*:\big) \\ & + \tilde{\omega}\big(:d_p c_q^* d_q^* c_p:\big) + \tilde{\omega}\big(:d_p d_q c_q c_p:\big) + \tilde{\omega}\big(:c_p^* d_q d_q^* d_p^*:\big) \\ & + \tilde{\omega}\big(:d_p c_q^* d_q^* d_p^*:\big) + \tilde{\omega}\big(:d_p d_q c_q d_p^*:\big) + \tilde{\omega}\big(:d_p d_q d_q^* c_p:\big) \\ & + \tilde{\omega}\big(:d_p d_q d_q^* d_p^*:\big) \Big\} \ . \end{aligned} \tag{5.249}$$

We divide the above expressions into four groups. Namely, we have

$$\tilde{\omega}\Big( \sum_{p,q\in\mathbb{N}} :a_p^* a_q^* a_q a_p: \Big) \ = \ \text{group 1} \ + \ \text{group 2} \ + \ \text{group 3} \ + \ \text{group 4} \ , \tag{5.250}$$

with

$$\text{group } 1 := \sum_{p,q\in\mathbb{N}} \Big\{\tilde\omega\big(c_q^* d_q^* d_p^* d_p\big) + \tilde\omega\big(d_q^* d_p d_q c_p\big) + \tilde\omega\big(d_p^* d_p d_q c_q\big) + \tilde\omega\big(c_p^* d_q^* d_p^* d_q\big)\Big\}\ , \tag{5.251}$$

$$\text{group } 2 := \sum_{p,q\in\mathbb{N}} \Big\{\tilde\omega\big(c_p^* c_q^* c_q c_p\big) + \tilde\omega\big(c_p^* c_q^* d_p^* c_q\big) + \tilde\omega\big(c_p^* c_q^* d_q^* c_p\big) + \tilde\omega\big(c_p^* d_q c_q c_p\big)$$
$$+ \tilde\omega\big(c_q^* d_p c_q c_p\big) + \tilde\omega\big(c_p^* d_q^* d_q c_p\big) + \tilde\omega\big(c_q^* d_p^* d_p c_q\big)\Big\}\ , \tag{5.252}$$

$$\text{group } 3 := \sum_{p,q\in\mathbb{N}} \Big\{\tilde\omega\big(c_p^* c_q^* d_q^* d_p^*\big) + \tilde\omega\big(d_p d_q c_q c_p\big)\Big\}\ ,$$

$$\text{group } 4 := \sum_{p,q\in\mathbb{N}} \Big\{\tilde\omega(c_q^* d_q^* d_p c_p) + \tilde\omega\big(c_q^* d_q^* d_p c_p\big) + \tilde\omega\big(d_q^* d_p^* d_p d_q\big)\Big\}\ . \tag{5.253}$$

We estimate these four groups separately.

$$\text{group } 1 = 4\,\mathrm{Re}\sum_{p,q\in\mathbb{N}} \tilde\omega(d_q^* d_p d_q c_p) \geq -4\sqrt{\sum_{p,q\in\mathbb{N}} \tilde\omega(d_q^* d_p d_p^* d_q)}\sqrt{\sum_{p,q\in\mathbb{N}} \tilde\omega(c_p^* d_q^* d_q c_p)}\ . \tag{5.254}$$

Here, we use just the Cauchy-Schwarz estimate.

$$\begin{aligned}
\text{group } 2 &= \sum_{p,q\in\mathbb{N}} \Big\{\tilde\omega(c_p^* c_q^* c_q c_p) + 4\,\mathrm{Re}\,\tilde\omega(c_q^* d_p c_q c_p) + 2\tilde\omega(c_q^* d_p^* d_p c_q)\Big\} \\
&\geq \sum_{p,q\in\mathbb{N}} \Big\{\tilde\omega(c_p^* c_q^* c_q c_p) - 4\sqrt{\tilde\omega(c_q^* d_p d_p^* c_q)}\sqrt{\tilde\omega(c_p^* c_q^* c_q c_p)} + 2\tilde\omega(c_q^* d_p^* d_p c_q)\Big\} \\
&= \sum_{p,q\in\mathbb{N}} \Big\{\Big[\sqrt{\tilde\omega(c_p^* c_q^* c_q c_p)} - 2\sqrt{\tilde\omega(c_q^* d_p d_p^* c_q)}\,\Big]^2 - 4\tilde\omega(c_q^* d_p d_p^* c_q) + 2\tilde\omega(c_q^* d_p^* d_p c_q)\Big\} \\
&\geq \sum_{p,q\in\mathbb{N}} \Big\{ - 4\,\big[d_p, d_p^*\big]\,\tilde\omega(c_q^* c_q) - 2\tilde\omega(c_q^* d_p^* d_p c_q)\Big\}\ .
\end{aligned} \tag{5.255}$$

Here, we first estimate using the Cauchy-Schwarz inequality. Then we complete a positive square, which we drop subsequently. In the last step, we commute $d_p$ with $d_p^*$. The two remaining quartic terms partially cancel each other.

$$\begin{aligned}
\text{group } 3 &= 2\,\mathrm{Re}\sum_{p,q\in\mathbb{N}} \tilde\omega(c_p^* c_q^* d_q^* d_p^*) = 2\,\mathrm{Re}\,\tilde\omega\bigg(\Big(\sum_{p\in\mathbb{N}} c_p^* d_p^*\Big)^2\bigg) \\
&\geq -2\sqrt{\sum_{p,q\in\mathbb{N}} \tilde\omega(c_p^* d_p^* d_q c_q)}\sqrt{\sum_{p,q\in\mathbb{N}} \tilde\omega(d_p c_p c_q^* d_q^*)}\ .
\end{aligned} \tag{5.256}$$

We use the Cauchy-Schwarz estimate. The expression under the second square root in the last line satisfies:

$$\begin{aligned}\sum_{p,q\in\mathbb{N}} \tilde{\omega}(d_p c_p c_q^* d_q^*) &= \sum_{p,q\in\mathbb{N}} \Big\{\tilde{\omega}(d_p c_q^* c_p d_q^*) + \big[c_p, c_q^*\big]\,\tilde{\omega}(d_p d_q^*)\Big\} \\ &= \sum_{p,q\in\mathbb{N}} \Big\{\tilde{\omega}(c_q^* d_p c_p d_q^*) + \big[d_p, c_q^*\big]\,\tilde{\omega}(c_p d_q^*) + \big[c_p, c_q^*\big]\,\tilde{\omega}(d_p d_q^*)\Big\} \\ &= \sum_{p,q\in\mathbb{N}} \Big\{\tilde{\omega}(c_q^* d_p d_q^* c_p) + \big[c_p, d_q^*\big]\,\tilde{\omega}(c_q^* d_p) + \big[d_p, c_q^*\big]\,\tilde{\omega}(d_q^* c_p) \qquad (5.257) \\ &\qquad + \big[d_p, c_q^*\big]\big[c_p, d_q^*\big] + \big[c_p, c_q^*\big]\big[d_p, d_q^*\big] + \big[c_p, c_q^*\big]\,\tilde{\omega}(d_q^* d_p)\Big\}\,.\end{aligned}$$

We are thus led to

$$\begin{aligned}\text{group } 3 \geq -2\sqrt{\sum_{p,q\in\mathbb{N}} \tilde{\omega}(c_p^* d_p^* d_q c_q)}\; \Big\{\sum_{p,q\in\mathbb{N}} \Big(&\tilde{\omega}(c_q^* d_q^* d_p c_p) + \big[d_p, d_q^*\big]\,\tilde{\omega}(c_q^* c_p) \\ &+ \big[c_p, d_q^*\big]\,\tilde{\omega}(c_q^* d_p) + \big[d_p, c_q^*\big]\,\tilde{\omega}(d_q^* c_p) + \big[d_p, c_q^*\big]\big[c_p, d_q^*\big] \\ &+ \big[c_p, c_q^*\big]\,\tilde{\omega}(d_q^* d_p) + \big[c_p, c_q^*\big]\big[d_p, d_q^*\big]\Big)\Big\}^{\frac{1}{2}}\,. \qquad (5.258)\end{aligned}$$

Finally, we exhaust all the sixteen terms by noting:

$$\text{group } 4 \geq 0\,. \qquad (5.259)$$

The next step we take is to estimate the four-point functions on the right hand sides of (5.254), (5.255) and (5.258), namely,

$$(i)\quad \sum_{p,q\in\mathbb{N}} \tilde{\omega}(c_p^* d_q^* d_q c_p)\quad,\qquad (ii)\quad \sum_{p,q\in\mathbb{N}} \tilde{\omega}(c_p^* d_p^* d_q c_q)\quad,\qquad (iii)\quad \sum_{p,q\in\mathbb{N}} \tilde{\omega}(d_q^* d_p d_p^* d_q) \qquad (5.260)$$

in terms of two-point functions (as far as we can). To this end, we note first:

$$\begin{aligned}\sum_{p,q\in\mathbb{N}} \tilde{\omega}(c_p^* d_p^* d_q c_q) &\leq \sum_{p,q\in\mathbb{N}} \big|\,\tilde{\omega}(c_p^* d_q d_p^* c_q)\,\big| + \Big|\sum_{p,q\in\mathbb{N}} \big[d_p^*, d_q\big]\,\tilde{\omega}(c_p^* c_q)\Big| \\ &\leq \sum_{p,q\in\mathbb{N}} \sqrt{\tilde{\omega}(c_p^* d_q d_q^* c_p)}\sqrt{\tilde{\omega}(c_q^* d_p d_p^* c_q)} + \Big|\sum_{p,q\in\mathbb{N}} \big[d_p^*, d_q\big]\,\tilde{\omega}(c_p^* c_q)\Big| \\ &\leq \sum_{p,q\in\mathbb{N}} \tilde{\omega}(c_p^* d_q d_q^* c_p) + \Big|\sum_{p,q\in\mathbb{N}} \big[d_p^*, d_q\big]\,\tilde{\omega}(c_p^* c_q)\Big| \\ &= \sum_{p,q\in\mathbb{N}} \Big\{\tilde{\omega}(c_p^* d_q^* d_q c_p) + \big[d_q, d_q^*\big]\,\tilde{\omega}(c_p^* c_p)\Big\} + \Big|\sum_{p,q\in\mathbb{N}} \big[d_p^*, d_q\big]\,\tilde{\omega}(c_p^* c_q)\Big|\,.\end{aligned} \qquad (5.261)$$

Here, we first commute $d_p^*$ with $d_p$, then use the triangle inequality and subsequently use the Cauchy-Schwarz inequality two times. In the resulting term, we again commute $d_q^*$ with $d_q$. This reduces the estimate of expression $(ii)$ to the estimate of expression $(i)$. The estimates of expressions $(i)$ and $(iii)$ are handled by the following two lemmas. (We postpone the proofs until after we complete the current proof on p. 137.)

**Lemma 5.26.** *Under the assumptions in Theorem 5.24 on the state $\omega$ and the Bogoliubov transformation $(w, v)$, we have:*

$$(i) = \sum_{p,q\in\mathbb{N}} \tilde{\omega}(c_p^* d_q^* d_q c_p) \leq 2\,\mathrm{tr}\left(\bar{D}^2 Y^* Y\right) \left[\| XD^2X^* \| \, \tilde{\omega}\left(\mathbf{n}^2\right) + \tilde{\omega}(\mathbf{n}) \, \| Du \|^2\right] . \tag{5.262}$$

**Lemma 5.27.** *Under the assumptions in Theorem 5.24 on the state $\omega$ and the Bogoliubov transformation $(w, v)$, we have:*

$$(iii) = \sum_{p,q\in\mathbb{N}} \tilde{\omega}(d_q^* d_p d_p^* d_q) \leq \mathrm{tr}\left(\bar{D}^2 Y^* Y\right)^2 \tilde{\omega}\left(\mathbf{n}^2\right) + \sum_{p,q\in\mathbb{N}} \left[d_p, d_p^*\right] \tilde{\omega}(d_q^* d_q) . \tag{5.263}$$

We have thus estimated all quartic expectation values in $\tilde{\omega}$ by quadratic ones and the expectation value $\tilde{\omega}(\mathbf{n}^2)$. We now insert these bounds into the estimates of groups 1-3 we have previously derived. From (5.254), we obtain

$$\begin{aligned} \text{group } 1 \geq -2^{\frac{5}{2}} &\left\{ \mathrm{tr}\left(\bar{D}^2 Y^* Y\right)^2 \tilde{\omega}\left(\mathbf{n}^2\right) + \sum_{p,q\in\mathbb{N}} \left[d_p, d_p^*\right] \tilde{\omega}(d_q^* d_q) \right\}^{\frac{1}{2}} \\ &\cdot \left\{ \mathrm{tr}\left(\bar{D}^2 Y^* Y\right) \left[\| XD^2X^* \| \, \tilde{\omega}\left(\mathbf{n}^2\right) + \tilde{\omega}(\mathbf{n}) \, \| Du \|^2\right] \right\}^{\frac{1}{2}} , \end{aligned} \tag{5.264}$$

where we make use of the estimates of the terms $(iii)$ and $(i)$. From (5.255), we obtain

$$\begin{aligned} \text{group } 2 \geq &-4 \sum_{p,q\in\mathbb{N}} \left[d_p, d_p^*\right] \tilde{\omega}(c_q^* c_q) \\ &- 4\,\mathrm{tr}\left(\bar{D}^2 Y^* Y\right) \left[\| XD^2X^* \| \, \tilde{\omega}\left(\mathbf{n}^2\right) + \tilde{\omega}(\mathbf{n}) \, \| Du \|^2\right] , \end{aligned} \tag{5.265}$$

using the estimate of $(i)$. From (5.258), we obtain

$$\begin{aligned} \text{group } 3 \geq -2 &\left\{ \sum_{p,q\in\mathbb{N}} \left[d_q, d_q^*\right] \tilde{\omega}(c_p^* c_p) + \left| \sum_{p,q\in\mathbb{N}} \left[d_q, d_p^*\right] \tilde{\omega}(c_p^* c_q) \right| \right. \\ &\left. \quad + \mathrm{tr}\left(\bar{D}^2 Y^* Y\right) \left[2 \, \| XD^2X^* \| \, \tilde{\omega}\left(\mathbf{n}^2\right) + 2\tilde{\omega}(\mathbf{n}) \, \| Du \|^2 \right] \right\}^{\frac{1}{2}} \\ &\cdot \left\{ \sum_{p,q\in\mathbb{N}} \Big( \left[c_p, d_q^*\right] \tilde{\omega}(c_q^* d_p) + \left[d_p, c_q^*\right] \tilde{\omega}(d_q^* c_p) + \left[c_p, c_q^*\right] \tilde{\omega}(d_q^* d_p) \right. \\ &\quad + \left[d_p, c_q^*\right] \left[c_p, d_q^*\right] + \left[c_p, c_q^*\right] \left[d_p, d_q^*\right] + \left[d_p, d_q^*\right] \tilde{\omega}(c_q^* c_p) \\ &\quad + \left[d_q, d_q^*\right] \tilde{\omega}(c_p^* c_p) \Big) + \left| \sum_{p,q\in\mathbb{N}} \left[d_q, d_p^*\right] \tilde{\omega}(c_p^* c_q) \right| \\ &\left. \quad + \mathrm{tr}\left(\bar{D}^2 Y^* Y\right) \left[2 \, \| XD^2X^* \| \, \tilde{\omega}\left(\mathbf{n}^2\right) + 2\tilde{\omega}(\mathbf{n}) \, \| Du \|^2\right] \right\}^{\frac{1}{2}} , \end{aligned} \tag{5.266}$$

where we have combined (5.261) and Lemma 5.26 to estimate expression $(ii)$.

We now provide explicit forms of the remaining two-point functions and commutators.

$$\sum_{p\in\mathbb{N}} \tilde{\omega}(d_p^* d_p) = \operatorname{tr}\left(\bar{D}^2 Y^* \tilde{\gamma} Y\right) \ , \tag{5.267a}$$

$$\sum_{p\in\mathbb{N}} \tilde{\omega}(c_p^* c_p) = \operatorname{tr}\left(D^2 X^* \tilde{\gamma} X\right) + 2\operatorname{Re}\left\langle \tilde{\delta} \,\middle|\, X D^2 u \right\rangle + \| \, Du \, \|^2 \ , \tag{5.267b}$$

$$\sum_{p\in\mathbb{N}} \left[d_p, d_p^*\right] = \operatorname{tr}\left(\bar{D}^2 Y^* Y\right) \ . \tag{5.267c}$$

Furthermore, we have for the following combinations:

$$\begin{aligned}\sum_{p,q\in\mathbb{N}} \left[d_q, d_p^*\right] \tilde{\omega}(c_p^* c_q) = {} & \operatorname{tr}\left(D^2 Y^T \bar{Y} D^2 X^* \tilde{\gamma} X\right) \\ & + 2\operatorname{Re}\left\langle u \,\middle|\, D^2 Y^T \bar{Y} D^2 X^* \tilde{\delta} \right\rangle + \left\langle u \,\middle|\, D^2 Y^T \bar{Y} D^2 u \right\rangle \ ,\end{aligned} \tag{5.267d}$$

$$\sum_{p,q\in\mathbb{N}} \left[c_p, d_q^*\right] \tilde{\omega}(c_q^* d_p) = \operatorname{tr}\left(D^2 Y^T \bar{X} \bar{D}^2 Y^* \tilde{\gamma} X\right) + \left\langle u \,\middle|\, D^2 Y^T \bar{X} \bar{D}^2 Y^* \tilde{\delta} \right\rangle \ , \tag{5.267e}$$

$$\sum_{p,q\in\mathbb{N}} \left[d_p, c_q^*\right] \tilde{\omega}(d_q^* c_p) = \operatorname{tr}\left(\bar{D}^2 X^T \bar{Y} D^2 X^* \tilde{\gamma} Y\right) + \left\langle \tilde{\delta} \,\middle|\, Y \bar{D}^2 X^T \bar{Y} D^2 u \right\rangle \ , \tag{5.267f}$$

$$\sum_{p,q\in\mathbb{N}} \left[c_p, c_q^*\right] \tilde{\omega}(d_q^* d_p) = \operatorname{tr}\left(D^2 X^* X D^2 Y^T \tilde{\gamma}^T \bar{Y}\right) \ , \tag{5.267g}$$

$$\sum_{p,q\in\mathbb{N}} \left[d_p, c_q^*\right] \left[c_p, d_q^*\right] = \operatorname{tr}\left(\bar{D}^2 Y^* X D^2 Y^T \bar{X}\right) \ , \tag{5.267h}$$

$$\sum_{p,q\in\mathbb{N}} \left[c_p, c_q^*\right] \left[d_p, d_q^*\right] = \operatorname{tr}\left(D^2 X^* X D^2 Y^T \bar{Y}\right) \ . \tag{5.267i}$$

Finally, we obtain the correlation estimate by inserting these expressions into the bounds we derived above. Inserting (5.267) into (5.264) yields:

$$\begin{aligned}\text{group 1} \geq -2^{\frac{5}{2}} \operatorname{tr}\left(\bar{D}^2 Y^* Y\right) & \left\{ \tilde{\omega}\left(\mathbf{n}^2\right) \operatorname{tr}\left(\bar{D}^2 Y^* Y\right) + \operatorname{tr}\left(\bar{D}^2 Y^* \gamma Y\right) \right\}^{\frac{1}{2}} \\ & \cdot \left\{ \| \, X D^2 X^* \, \| \, \tilde{\omega}\left(\mathbf{n}^2\right) + \tilde{\omega}(\mathbf{n}) \, \| \, Du \, \|^2 \right\}^{\frac{1}{2}} \ .\end{aligned} \tag{5.268}$$

Inserting (5.267) into (5.265) yields

$$\begin{aligned}\text{group 2} \geq -4 \operatorname{tr}\left(\bar{D}^2 Y^* Y\right) \Big[ & \operatorname{tr}\left(D^2 X^* \tilde{\gamma} X\right) + 2\operatorname{Re}\left\langle \delta_\omega \,\middle|\, X D^2 u \right\rangle + \| \, Du \, \|^2 \\ & + \| \, X D^2 X^* \, \| \, \tilde{\omega}\left(\mathbf{n}^2\right) + \tilde{\omega}(\mathbf{n}) \, \| \, Du \, \|^2 \Big] \ .\end{aligned} \tag{5.269}$$

Inserting (5.267) into (5.266) yields

$$\begin{aligned}\text{group } 3 \geq -2\Big\{ &\operatorname{tr}\left(\bar{D}^2 Y^* Y\right)\Big[2\operatorname{Re}\left\langle \tilde{\delta} \,\middle|\, X D^2 u \right\rangle + \|\, Du \,\|^2 + 2\operatorname{tr}\left(D^2 X^* \tilde{\gamma} X\right) \\ &+ 2\tilde{\omega}(\mathbf{n}) \,\|\, Du \,\|^2 + 2 \,\big\|\, X D^2 X^* \,\big\|\, \tilde{\omega}\left(\mathbf{n}^2\right)\Big] + 2\left|\left\langle u \,\middle|\, D^2 Y^T \bar{Y} D^2 X^* \tilde{\delta} \right\rangle\right| \\ &+ \left\langle u \,\middle|\, D^2 Y^T \bar{Y} D^2 u \right\rangle \Big\}^{\frac{1}{2}} \\ \cdot\Big\{ &2 \left|\operatorname{tr}\left(D^2 Y^T \bar{X} \bar{D}^2 Y^* \tilde{\gamma} X\right)\right| + 2\left|\left\langle u \,\middle|\, D^2 Y^T \bar{X} \bar{D}^2 Y^* \tilde{\delta} \right\rangle\right| \\ &+ \operatorname{tr}\left(\bar{D}^2 Y^* X D^2 Y^T \bar{X}\right) + \operatorname{tr}\left(D^2 X^* X D^2 Y^T (\mathbf{1} + \tilde{\gamma}^T) \bar{Y}\right) \\ &+ 4\left|\left\langle u \,\middle|\, D^2 Y^T \bar{Y} D^2 X^* \tilde{\delta} \right\rangle\right| + 2\left\langle u \,\middle|\, D^2 Y^T \bar{Y} D^2 u \right\rangle \\ &+ \operatorname{tr}\left(\bar{D}^2 Y^* Y\right)\Big[2\operatorname{Re}\left\langle \tilde{\delta} \,\middle|\, X D^2 u \right\rangle + \|\, Du \,\|^2 + 3\operatorname{tr}\left(D^2 X^* \tilde{\gamma} X\right) \\ &+ 2\tilde{\omega}(\mathbf{n}) \,\|\, Du \,\|^2 + 2 \,\big\|\, X D^2 X^* \,\big\|\, \tilde{\omega}\left(\mathbf{n}^2\right)\Big]\Big\}^{\frac{1}{2}} \ . \end{aligned} \tag{5.270}$$

Additionally to inserting (5.267), we have estimated

$$\begin{aligned}\operatorname{tr}\left(D^2 Y^T \bar{Y} D^2 X^* \tilde{\gamma} X\right) &\leq \sqrt{\operatorname{tr}\left((D Y^T \bar{Y} D)^2\right)}\sqrt{\operatorname{tr}\left((D X^* \tilde{\gamma} X)^2\right)} \\ &\leq \operatorname{tr}\left(\bar{D}^2 Y^* Y\right) \operatorname{tr}\left(D^2 X^* \gamma X\right) \ . \end{aligned} \tag{5.271}$$

We arrive at the claim of the theorem by summing up the estimates (5.268), (5.269) and (5.270), see (5.250). □

We now present the proofs of the two lemmas we have used.

*Proof of Lemma 5.26:* First we note that, by the Cauchy-Schwarz estimate, we have for the left hand side (l. h. s.) of the claim (5.262):

$$\begin{aligned}\text{l. h. s.} &= \sum_{p,q\in\mathbb{N}} \tilde{\omega}(c_p^* d_q^* d_q c_p) = \sum_{p,q\in\mathbb{N}} \tilde{\omega}\big(c_p^* a^*(Y\overline{D f_q}) a(Y\overline{D f_q}) c_p\big) \\ &= \sum_{p,q\in\mathbb{N}} \sum_{k,l\in\mathbb{N}} (Y\bar{D})_{l,q} (\bar{Y} D)_{k,q}\, \tilde{\omega}\big(c_p^* a^*(\bar{f}_l) a(\bar{f}_k) c_p\big) \\ &= \sum_{p\in\mathbb{N}} \sum_{k,l\in\mathbb{N}} (Y\bar{D}^2 Y^*)_{l,k} \tilde{\omega}\big(c_p^* a^*(\bar{f}_l) a(\bar{f}_k) c_p\big) \\ &\leq \sum_{p\in\mathbb{N}} \sqrt{\sum_{k,l\in\mathbb{N}} \left|\, (Y\bar{D}^2 Y^*)_{l,k} \,\right|^2} \sqrt{\sum_{k,l\in\mathbb{N}} \left|\, \tilde{\omega}\big(c_p^* a^*(\bar{f}_l) a(\bar{f}_k) c_p\big) \,\right|^2} \ . \end{aligned} \tag{5.272}$$

Thus we obtain

$$\text{l. h. s.} \leq \operatorname{tr}\left(\bar{D}^2 Y^* Y\right) \sum_{p\in\mathbb{N}} \tilde{\omega}(c_p^* \,\mathbf{n}\, c_p) \ . \tag{5.273}$$

Let us now calculate the second factor in the above expression. Inserting (5.247) yields

$$\sum_{p\in\mathbb{N}} \tilde{\omega}(c_p^* \, \mathbf{n} \, c_p) = \sum_{p\in\mathbb{N}} \Big[ \tilde{\omega}\big(a^*(XDf_p) \, \mathbf{n} \, a(XDf_p)\big) + 2\,\mathrm{Re}\left( \tilde{\omega}\big(a^*(XDf_p) \, \mathbf{n}\,\big) \langle Df_p \,|\, u \rangle \right) + \tilde{\omega}(\mathbf{n}) \left| \langle u \,|\, Df_p \rangle \right|^2 \Big] . \tag{5.274}$$

As far as the first term on the right hand side of the last equation is concerned, we proceed similarly as in the previous estimate. Namely, we have

$$\sum_{p\in\mathbb{N}} \tilde{\omega}\big(a^*(XDf_p) \, \mathbf{n} \, a(XDf_p)\big) = \sum_{k,l\in\mathbb{N}} (XD^2X^*)_{k,l} \, m_{l,k} \ , \tag{5.275}$$

for the nonnegative operator $m$ in $\mathcal{H}^1$ given by

$$m_{l,k} := \langle f_l \,|\, m f_k \rangle = \tilde{\omega}\big(a^*(f_k) \, \mathbf{n} \, a(f_l)\big) \quad , \qquad \forall \ k,l \in \mathbb{N} \ . \tag{5.276}$$

With this notation we may write:

$$\sum_{p\in\mathbb{N}} \tilde{\omega}(c_p^* \, \mathbf{n} \, c_p) \leq \mathrm{tr}\left( m^{\frac{1}{2}} XD^2X^* m^{\frac{1}{2}} \right) + 2 \sqrt{\tilde{\omega}\left(\mathbf{n}^2\right) \sum_{p\in\mathbb{N}} \tilde{\omega}\big(a^*(XDf_p) a(XDf_p)\big)} \, \| \, Du \, \| + \tilde{\omega}(\mathbf{n}) \, \| \, Du \, \|^2 \ , \tag{5.277}$$

where we have used the Cauchy-Schwarz estimate three times on the middle term and we have also used Parseval's equality. We must now avoid to use the Cauchy-Schwarz inequality to estimate the first of the terms in this expression, since $X$ will in general not be trace-class. Instead, we estimate

$$\mathrm{tr}\left( m^{\frac{1}{2}} XD^2X^* m^{\frac{1}{2}} \right) \leq \left\| \, XD^2X^* \, \right\| \mathrm{tr}(m) = \left\| \, XD^2X^* \, \right\| \tilde{\omega}\big( \, \mathbf{n}(\mathbf{n} - \mathbf{1})\big) \ . \tag{5.278}$$

Thus it holds true that

$$\begin{aligned} \sum_{p\in\mathbb{N}} \tilde{\omega}(c_p^* \, \mathbf{n} \, c_p^*) &\leq \left\| \, XD^2X^* \, \right\| \tilde{\omega}\big( \, \mathbf{n}(\mathbf{n} - \mathbf{1})\big) \\ &\qquad + 2 \sqrt{\tilde{\omega}\left(\mathbf{n}^2\right) \sum_{p\in\mathbb{N}} \tilde{\omega}\big(a^*(XDf_p) a(XDf_p)\big)} \, \| \, Du \, \| + \tilde{\omega}(\mathbf{n}) \, \| \, Du \, \|^2 \\ &\leq \left\| \, XD^2X^* \, \right\| \tilde{\omega}\big( \, \mathbf{n}(\mathbf{n} - \mathbf{1})\big) \\ &\qquad + 2 \sqrt{\tilde{\omega}\left(\mathbf{n}^2\right) \| \, XD^2X^* \, \| \, \tilde{\omega}(\mathbf{n})} \ \| \, Du \, \| + \tilde{\omega}(\mathbf{n}) \, \| \, Du \, \|^2 \\ &\leq 2 \left\| \, XD^2X^* \, \right\| \tilde{\omega}\left(\mathbf{n}^2\right) + 2\tilde{\omega}(\mathbf{n}) \, \| \, Du \, \|^2 \ . \end{aligned} \tag{5.279}$$

In the second last step, we have estimated, similarly as above,

$$\sum_{p\in\mathbb{N}} \tilde{\omega}\big(a^*(XDf_p) a(XDf_p)\big) \leq \left\| \, XD^2X^* \, \right\| \tilde{\omega}(\mathbf{n}) \ . \tag{5.280}$$

Then we have used the elementary estimate

$$2ab \ \leq \ a^2 + b^2 \quad , \qquad \forall \ a,b \in \mathbb{R} \ . \tag{5.281}$$

(5.273) and (5.279) prove the claim of the lemma. ☐

*Proof of Lemma 5.27:* For the left hand side (l. h. s.) of the claim (5.263), we have

$$\text{l. h. s.} = \sum_{p,q\in\mathbb{N}} \tilde{\omega}(d_q^* d_p d_p^* d_q) = \sum_{p,q\in\mathbb{N}} \tilde{\omega}(d_q^* d_p^* d_p d_q) + \sum_{p,q\in\mathbb{N}} \big[d_p, d_p^*\big]\, \tilde{\omega}(d_q^* d_q) \ . \tag{5.282}$$

We continue estimating as follows:

$$\begin{aligned} \sum_{p,q\in\mathbb{N}} \tilde{\omega}(d_q^* d_p^* d_p d_q) &= \sum_{q\in\mathbb{N}} \sum_{k,l\in\mathbb{N}} (Y\bar{D}D^T Y^*)_{k,l}\, \tilde{\omega}(d_q^* a^*(\bar{f}_k) a(\bar{f}_l) d_q) \\ &\le \sum_{q\in\mathbb{N}} \sqrt{\sum_{k,l\in\mathbb{N}} \big|\, (Y\bar{D}^2 Y^*)_{k,l}\, \big|^2} \sqrt{\sum_{k,l\in\mathbb{N}} \big|\, \tilde{\omega}\big(d_q^* a^*(\bar{f}_k) a(\bar{f}_l) d_q\big)\, \big|^2} \\ &\le \operatorname{tr}\big(\bar{D}^2 Y^* Y\big) \sum_{q\in\mathbb{N}} \tilde{\omega}(d_q^*\, \mathbf{n}\, d_q) \ , \end{aligned} \tag{5.283}$$

where we have used the same technique as in (5.273). This yields

$$\text{l. h. s.} \le \operatorname{tr}\big(\bar{D}^2 Y^* Y\big) \sum_{q\in\mathbb{N}} \tilde{\omega}(d_q^*\, \mathbf{n}\, d_q) + \sum_{p,q\in\mathbb{N}} \big[d_p, d_p^*\big]\, \tilde{\omega}(d_q^* d_q) \ . \tag{5.284}$$

The remaining quartic term $\tilde{\omega}(d_q^*\, \mathbf{n}\, d_q)$ is somewhat easier to estimate as the corresponding term involving the $c$'s, since $Y^*Y$ is trace-class, if the Bogoliubov transformation $(w, v)$ possesses a unitary implementation. Hence, we can estimate

$$\begin{aligned} \sum_{q\in\mathbb{N}} \tilde{\omega}(d_q^*\, \mathbf{n}\, d_q) &= \sum_{k,l\in\mathbb{N}} (Y\bar{D}^2 Y^*)_{k,l}\, \tilde{\omega}\big(a^*(\bar{f}_k)\, \mathbf{n}\, a(\bar{f}_l)\big) \le \operatorname{tr}\big((Y\bar{D}^2 Y^*)^2\big)^{\frac{1}{2}} \operatorname{tr}\big(m^2\big)^{\frac{1}{2}} \\ &\le \operatorname{tr}\big(\bar{D}^2 Y^* Y\big) \operatorname{tr}(m) = \operatorname{tr}\big(\bar{D}^2 Y^* Y\big)\, \tilde{\omega}\big(\, \mathbf{n}(\mathbf{n} - \mathbf{1})\big) \le \operatorname{tr}\big(\bar{D}^2 Y^* Y\big)\, \tilde{\omega}\, \big(\mathbf{n}^2\big) \ , \end{aligned} \tag{5.285}$$

where we have denoted

$$m_{l,k} := \tilde{\omega}\big(a^*(\bar{f}_k)\, \mathbf{n}\, a(\bar{f}_l)\big) \quad , \qquad \forall\ k, l \in \mathbb{N} \ . \tag{5.286}$$

This last observation together with (5.282) and (5.284) proves the claim. ☐

# Appendix A

# Definitizable Operators in Krein Spaces

In this appendix, we briefly review the elements of the theory of linear operators in Krein spaces needed for our considerations and we prove Lemma 3.12. Proofs of the following theorems can mostly be found in [22]. Other references to this topic are [4] and [12].

## A.1 Fundamentals

**Definition A.1.** *Let $V$ be a complex linear space. A hermitian sesqui-linear form on $V$ (linear in the second entry)*

$$[\cdot\,|\,\cdot] : V \times V \longrightarrow \mathbb{C} \ , \tag{A.1}$$

*which is nondegenerate, i. e., which fulfills*

$$\big(\, [x\,|\,y] = 0 \ , \quad \forall\, y \in V \,\big) \quad \Rightarrow \quad x = 0 \ , \tag{A.2}$$

*for all $x \in V$, is called an* <u>*inner product*</u> *on $V$. If a linear space $V$ is equipped with such an inner product, it is called an* <u>*inner product space*</u>*. Vectors in $V$ having positive, respectively negative inner product with themselves are called* <u>*positive vectors*</u>*, respectively* <u>*negative vectors*</u>*. Elements of $V$ having vanishing inner product with themselves are called* <u>*neutral vectors*</u>*.*

Note that in $V$ there may or may not exist positive or negative vectors, respectively. The zero vector is always neutral, but there may be more then just one neutral vector. Accordingly, we define the following attributes for any inner product space $V$.

- $V$ is said to be a <u>nonnegative inner product space</u>, if none of its vectors is negative.
- $V$ is said to be a <u>positive inner product space</u>, if all vectors but the zero vector are positive.
- $V$ is said to be a <u>nonpositive inner product space</u>, if none of its vectors is positive.

- $V$ is said to be a negative inner product space, if all vectors but the zero vector are negative.
- $V$ is said to be an indefinite inner product space, if it is neither nonnegative nor nonpositive.

**Definition A.2.** *An inner product space $\mathcal{K}$ admitting a decomposition into a direct sum $\mathcal{K} = \mathcal{K}_+ \oplus \mathcal{K}_-$ of subspaces $\mathcal{K}_+$ and $\mathcal{K}_-$, which obey the orthogonality condition*

$$[x \,|\, y] = 0 \quad , \qquad \forall\; x \in \mathcal{K}_+,\; y \in \mathcal{K}_- \;, \tag{A.3}$$

*such that each of the decomposition subspaces $\mathcal{K}_\pm$ is a Hilbert space together with the scalar product $\pm[\cdot\,|\,\cdot]\restriction_{\mathcal{K}_\pm}$, is called a Krein space. The above decomposition is then called a fundamental decomposition and is denoted by*

$$\mathcal{K} = \mathcal{K}_+ {}^{[+]}\, \mathcal{K}_- \;. \tag{A.4}$$

Obviously, any positive Krein space is in fact a Hilbert space. Note, on the other hand, that an indefinite Krein space $\mathcal{K}$ may admit more than one fundamental decomposition. It can be shown, however, that, for any two fundamental decompositions, the positive decomposition subspaces are unitarily equivalent as Hilbert spaces. The same is of course true for the negative decomposition subspaces.

Given a fixed fundamental decomposition of the form (A.4), we may uniquely decompose any vector $x$ in $\mathcal{K}$ according to

$$x = x_+ + x_- \qquad \text{such that} \qquad x_\pm \in \mathcal{K}_\pm \;. \tag{A.5}$$

This defines the fundamental projections $P_+$ and $P_-$ associated to the fundamental decomposition (A.4), simply by

$$P_\pm x := x_\pm \quad , \qquad \forall\; x \in \mathcal{K} \;. \tag{A.6}$$

It is then easy to see that

$$\langle x \,|\, y \rangle := [x \,|\, \eta y] \quad , \qquad \forall\; x, y \in \mathcal{K} \quad , \quad \text{with} \qquad \eta := P_+ - P_- \;, \tag{A.7}$$

defines a scalar product on $\mathcal{K}$. The everywhere defined operator $\eta$ is called a fundamental symmetry and depends of course on the fundamental decomposition. Furthermore, we note that, with respect to this scalar product, the fundamental decomposition (A.4) is also an orthogonal direct sum and

$$\langle x \,|\, y \rangle = [x_+ \,|\, y_+] - [x_- \,|\, y_-] \quad , \qquad \forall\; x, y \in \mathcal{K} \;. \tag{A.8}$$

Thus $(\mathcal{K}, \langle \cdot \,|\, \cdot \rangle)$ is a Hilbert space and we denote the induced norm simply by $\|\cdot\|$. In particular $\mathcal{K}$ is complete with respect to any norm arising in this way. Since $\eta^2 = \mathbf{1}$, the following property of the fundamental symmetry may be directly verified:

$$\|\, \eta x \,\|^2 = [\eta x \,|\, x] = [x \,|\, \eta x] = \|\, x \,\|^2 \quad , \qquad \forall\; x \in \mathcal{K} \;. \tag{A.9}$$

This implies

$$|\, [y \,|\, x] \,| = |\, \langle y \,|\, \eta x \rangle \,| \le \|\, y \,\| \,\|\, \eta x \,\| = \|\, y \,\| \,\|\, x \,\| \quad , \qquad \forall\; x, y \in \mathcal{K} \;, \tag{A.10}$$

and hence the inner product is continuous with respect to the Hilbert space norm.

All the topological and Banach space notions we shall shortly introduce, are always defined with respect to this Hilbert space norm. As it seems, all these statements depend on the fundamental decomposition chosen in (A.4). This is not so! It turns out that, if we had chosen a different fundamental decomposition, we would have obtained an equivalent norm. Thus the resulting topology on $\mathcal{K}$ is independent of this choice. We prove this fact.

**Theorem A.3.** *Any two Banach space norms $\|\cdot\|_1$ and $\|\cdot\|_2$ on $\mathcal{K}$, with the property that the inner product is continuous with respect to both of them, are equivalent.*

Since the hypothesis of this theorem is satisfied for all norms associated to a fundamental decomposition, as we have seen above, all such norms are equivalent. We shall therefore refer to *the* norm $\|\cdot\|$ without making any reference to any fundamental decomposition.

*Proof of Theorem A.3:* Consider a third norm $\|\cdot\|_3$ on $\mathcal{K}$, defined by

$$\| x \|_3 := \| x \|_1 + \| x \|_2 \quad , \qquad \forall\, x \in \mathcal{K} \ . \tag{A.11}$$

Suppose $\{x_n\}_{n\in\mathbb{N}}$ was a Cauchy sequence with respect to $\|\cdot\|_3$. It is then also a Cauchy sequence with respect to $\|\cdot\|_1$ and $\|\cdot\|_2$, and thus

$$\left\| x_n - x^{(1)} \right\|_1 \xrightarrow{n\to\infty} 0 \qquad \text{and} \qquad \left\| x_n - x^{(2)} \right\|_2 \xrightarrow{n\to\infty} 0 \ , \tag{A.12}$$

for some $x^{(1)}$ and $x^{(2)}$ in $\mathcal{K}$. Continuity of the inner product with respect to both of these norms, implies

$$\left[ x_n - x^{(1)} \,|\, y \right] \xrightarrow{n\to\infty} 0 \qquad \text{and} \qquad \left[ x_n - x^{(2)} \,|\, y \right] \xrightarrow{n\to\infty} 0 \ , \tag{A.13}$$

for all $y \in \mathcal{K}$. This in turn implies

$$\left[ x^{(1)} - x^{(2)} \,|\, y \right] = 0 \quad , \qquad \forall\, y \in \mathcal{K} \tag{A.14}$$

and, by assumed non-degeneracy of the inner product, we have $x^{(3)} := x^{(1)} = x^{(2)}$. Therefore

$$\left\| x_n - x^{(3)} \right\|_3 \xrightarrow{n\to\infty} 0 \ . \tag{A.15}$$

This shows that $\|\cdot\|_3$ is also a Banach space norm on $\mathcal{K}$. Let $\iota \in \{1, 2\}$. Clearly $\|\cdot\|_3$ dominates $\|\cdot\|_\iota$ and therefore the identity is a continuous mapping from $(\mathcal{K}, \|\cdot\|_3)$ onto $(\mathcal{K}, \|\cdot\|_\iota)$. By the inverse mapping theorem, its inverse (!) is also continuous and therefore $\|\cdot\|_\iota$ also dominates $\|\cdot\|_3$. We have thus shown that $\|\cdot\|_1$ and $\|\cdot\|_2$ are both equivalent to $\|\cdot\|_3$, thus proving the theorem. □

## A.2 Some Classes of Linear Operators in Krein Spaces

Let us now consider some Krein space $\mathcal{K}$, additionally equipped with a norm $\|\cdot\|$, a scalar product $\langle\cdot\,|\,\cdot\rangle$ and a fundamental symmetry $\eta$ arising, as described in the previous section, from a fundamental decomposition.

Let $A$ be a linear operator in $\mathcal{K}$, defined on some domain $\mathcal{D}(A)$. We say that $A$ is a bounded operator if

$$\| A \| := \sup_{\psi \in \mathcal{D}(A),\ \| x \| = 1} \| Ax \| < \infty \tag{A.16}$$

introducing the norm of the operator $A$, denoted by $\| A \|$. The set of all bounded operators defined on the whole of $\mathcal{K}$ is denoted by $\mathcal{B}(\mathcal{K})$.

Analogously to the Hilbert space case, we define a Krein space adjoint of a densely defined operator $A$, denoted by $A^{[*]}$, by first specifying its domain

$$\mathcal{D}\big(A^{[*]}\big) := \Big\{ x \in \mathcal{K} \mid \exists\, x' \in \mathcal{K},\ \forall\, y \in \mathcal{D}(A) :\ [Ay \,|\, x] = \big[y \,\big|\, x'\big] \Big\} . \tag{A.17}$$

Note that by the density assumption on the domain of $A$ and by the continuity and non-degeneracy of the inner product, the $x'$ above is unique, if it exists. On that domain, $A^{[*]}$ is thus uniquely determined by

$$[Ay \,|\, x] = \big[y \,\big|\, A^{[*]}x\big] \quad , \qquad \forall\, y \in \mathcal{D}(A),\ x \in \mathcal{D}(A^{[*]}) . \tag{A.18}$$

Denoting the adjoint of $A$ with respect to the scalar product $\langle \cdot \,|\, \cdot \rangle$ by $A^*$, we find

$$[Ax \,|\, y] = \langle Ax \,|\, \eta y \rangle = \langle x \,|\, A^* \eta y \rangle = \langle x \,|\, \eta(\eta A^* \eta) y \rangle = [x \,|\, \eta A^* \eta y] \ , \tag{A.19}$$

for all $x \in \mathcal{D}(A)$ and $y \in \eta\mathcal{D}(A^*)$. We are thus led to the conclusion that

$$\mathcal{D}(A^*) = \eta \mathcal{D}(A^{[*]}) \qquad \text{and} \qquad A^{[*]} = \eta A^* \eta . \tag{A.20}$$

Let us introduce the following classes of linear, densely defined operators.

- An operator $A$, defined on the whole of $\mathcal{K}$, is called isometric in the Krein space, if

$$[Ax \,|\, Ay] = [x \,|\, y] \quad , \qquad \forall\, x, y \in \mathcal{K} . \tag{A.21}$$

- An operator $A$ is called unitary in the Krein space, if

$$A^{[*]}A = AA^{[*]} = \mathbf{1} , \tag{A.22}$$

  implying that $\mathcal{D}(A) = \mathcal{D}(A^{[*]}) = \mathcal{K}$.

- A densely defined operator $A$ is called selfadjoint in the Krein space if

$$A^{[*]} = A , \tag{A.23}$$

  implying $\mathcal{D}(A) = \mathcal{D}(A^{[*]})$.

- An operator $E \in \mathcal{B}(\mathcal{K})$ is called an orthogonal projection in the Krein space, if it is selfadjoint in the Krein space and fulfills, furthermore, $E^2 = E$. ($\| E \| > 1$ is possible!)

Along the same lines as in the Hilbert space case, it is possible to prove, for any operator $A$ in $\mathcal{K}$:

$$A \text{ isometric and surjective } \Leftrightarrow\ A \text{ unitary} \tag{A.24}$$

Somewhat more difficult to prove is the fact that any unitary operator in the Krein space is also bounded. Since this is a very important statement in our context, we shall present the proof.

**Theorem A.4.** *Let $\mathcal{K}$ be a Krein space admitting a fundamental decomposition*

$$\mathcal{K} = \mathcal{K}_+ {}^{[+]}\, \mathcal{K}_- \tag{A.25}$$

*which defines the norm $\|\cdot\|$ on $\mathcal{K}$. Furthermore, let $w$ be a unitary operator in $\mathcal{K}$. Then the following statements hold true:*

*(i) Setting $\tilde{\mathcal{K}}_\pm := w\mathcal{K}_\pm$, we obtain a fundamental decomposition*

$$\mathcal{K} = \tilde{\mathcal{K}}_+ {}^{[+]}\, \tilde{\mathcal{K}}_- \ . \tag{A.26}$$

*(ii) $w$ is bounded.*

*Proof:* (i) Let $x$ be an arbitrary vector in $\mathcal{K}$. Then we can decompose

$$w^{[*]}x = (w^{[*]}x)_+ + (w^{[*]}x)_- \qquad \text{such that} \qquad (w^{[*]}x)_\pm \in \mathcal{K}_\pm \ . \tag{A.27}$$

Hence we have by unitarity

$$x = ww^{[*]}x = w(w^{[*]}x)_+ + w(w^{[*]}x)_- \ . \tag{A.28}$$

By construction $w(w^{[*]}x)_\pm \in \tilde{\mathcal{K}}_\pm$ follows. Furthermore, it follows, for any $x \in \tilde{\mathcal{K}}_+ \cap \tilde{\mathcal{K}}_-$, that there exist $y_+ \in \mathcal{K}_+$ and $y_- \in \mathcal{K}_-$ such that

$$x = wy_+ = wy_- \ . \tag{A.29}$$

By the isometry relation $w^{[*]}w = \mathbf{1}$, this implies $y_+ = y_-$ and thus $y = 0$, since (A.25) is a direct sum. Hence it follows that $x = 0$. Therefore

$$\tilde{\mathcal{K}}_+ \cap \tilde{\mathcal{K}}_- = \{0\} \ . \tag{A.30}$$

We have thus shown that (A.26) is a direct sum. The orthogonality condition follows from

$$[x \,|\, y] = [wx_+ \,|\, wy_-\,] = [x_+ \,|\, y_-\,] = 0 \ , \tag{A.31}$$

for $x := wx_+$ and any $y := wy_-$, where $x_+$ and $y_-$ are arbitrary elements of $\mathcal{K}_+$ and $\mathcal{K}_-$. The Hilbert space property of $\tilde{\mathcal{K}}_\pm$ with respect to the inner product $\pm[\cdot\,|\,\cdot]\restriction_{\tilde{\mathcal{K}}_\pm}$ follows similarly.

(ii) Denote by $\|\cdot\|_1$ the norm associated to the fundamental decomposition (A.26). Since it is equivalent to the norm $\|\cdot\|$ associated to (A.25), we may infer, by Theorem A.3:

$$\begin{aligned} \|\, wx \,\|^2 \leq c \,\|\, wx \,\|_1^2 = c \left( [wx_+ \,|\, wx_+] - [wx_- \,|\, wx_-\,] \right) = \\ = c \left( [x_+ \,|\, x_+] - [x_- \,|\, x_-\,] \right) = c \,\|\, x \,\|^2 \ , \end{aligned} \tag{A.32}$$

for some $c > 0$ and all $x \in \mathcal{K}$ with

$$x = x_+ + x_- \qquad \text{such that} \qquad x_\pm \in \mathcal{K}_\pm \ . \tag{A.33}$$

This completes our proof. $\square$

*Alternative proof of Theorem A.4 (ii):* It suffices to show that $w^{[*]}$ is bounded, because the inverse mapping theorem then implies that $w$ is also bounded. Furthermore, by the closed graph theorem, it suffices to show that $w^{[*]}$ is closed.

Suppose we are given a sequence $\{x_n\}_{n\in\mathbb{N}}$ in $\mathcal{K}$ such that

$$x_n \xrightarrow{n\to\infty} x \qquad \text{and} \qquad w^{[*]}x_n \xrightarrow{n\to\infty} y \ , \tag{A.34}$$

for some $x, y \in \mathcal{K}$, in the norm topology. It then follows from the continuity of the inner product that

$$[wz\,|\,x] = \lim_{n\to\infty}[wz\,|\,x_n] = \lim_{n\to\infty}\left[z\,\middle|\,w^{[*]}x_n\right] = [z\,|\,y] \quad , \qquad \forall\ z \in \mathcal{K}\ . \tag{A.35}$$

This implies $[z\,|\,w^{[*]}x - y] = 0$ for all $z \in \mathcal{K}$. By the nondegeneracy of the inner product this implies $w^{[*]}x = y$. Hence $w^{[*]}$ is closed. □

A striking difference compared to the Hilbert space case is that general closed subspaces $V$ of $\mathcal{K}$ are general inner product spaces, not necessarily Krein spaces. An important statement is the following theorem, providing a necessary and sufficient condition for $V$ to be itself a Krein space. For a proof, we refer the reader to Theorem I.5.2 in [22].

**Theorem A.5.** *Let $V \subseteq \mathcal{K}$ be a closed subspace. Then $V$ is itself a Krein space together with the inner product $[\cdot\,|\,\cdot]\restriction_V$, if and only if*

$$V = E\mathcal{K}\ , \tag{A.36}$$

*for some orthogonal projection $E$ in the Krein space $\mathcal{K}$.*

## A.3 Definitizable Operators in Krein Space

We say that an operator $A$ in $\mathcal{K}$, defined on $\mathcal{D}(A)$, is a nonnegative operator, if

$$[x\,|\,Ax] \geq 0 \qquad\qquad \forall\ x \in \mathcal{D}(A)\ . \tag{A.37}$$

We say that the operator $A$ is a uniformly positive operator, if there exists an $\varepsilon > 0$ such that

$$[x\,|\,Ax] \geq \varepsilon\,\|\,x\,\|^2 \qquad\qquad \forall\ x \in \mathcal{D}(A)\ . \tag{A.38}$$

The aim of this section is to prove Lemma 3.12. Due to the admissibility condition, the only case we are interested in, is the case of bounded and everywhere defined operators in $\mathcal{K}$.

An important property of nonnegative operators in $\mathcal{B}(\mathcal{K})$ is that they have real spectrum, only. (See Theorem VII.1.3 in [12].) This is, in marked contrast to the Hilbert space case, generally not true for all selfadjoint operators in $\mathcal{B}(\mathcal{K})$.

**Definition A.6.** *A selfadjoint operator $A \in \mathcal{B}(\mathcal{K})$ is said to be definitizable, if there exists a real*[1] *polynomial $p$ such that*

$$[x \,|\, p(A)x] \geq 0 \quad , \qquad \forall\, x \in \mathcal{K} \ , \tag{A.39}$$

*i. e., such that $p(A)$ is nonnegative. In this case the polynomial $p$ is called a definitizing polynomial of $A$.*

Obviously, nonnegative operators in $\mathcal{B}(\mathcal{K})$ are definitizable by the definitizing polynomial $id$. The spectrum of any selfadjoint, definitizable operator $A \in \mathcal{B}(\mathcal{K})$ is always contained in $\mathbb{R} \cup C$, where $C$ is a finite subset of $\mathbb{C}$.

A treatment of selfadjoint, definitizable operators in Krein spaces completely analogous to the Hilbert space case is possible, if the operator in question possesses no critical points. The set of critical points $c(A)$ of an operator $A = A^{[*]} \in \mathcal{B}(\mathcal{K})$ is defined in the following way:

$$c(A) := \left( \bigcap_{p \text{ definitizing}} N(p) \right) \cap \sigma(A) \cap \mathbb{R} \ . \tag{A.40}$$

The first set on the right hand side is the set of zeros common to all definitizing polynomials of $A$. Obviously, zero is the only possible critical point of a bounded operator, which is nonnegative.

As a preparation to the main theorem of this section, we define to any definitizable operator $A$ the semi-ring $\mathcal{R}_A$ generated by all bounded intervals in $\mathbb{R}$ and their complements in $\mathbb{R}$, with endpoints not in $c(A)$. This allows us to formulate (see Theorem II.3.1 in [22]):

**Theorem A.7.** *Let a definitizable operator $A \in \mathcal{B}(\mathcal{K})$ with real spectrum be given. Then there exists a mapping $E : \mathcal{R}_A \to \mathcal{B}(\mathcal{K})$, called the spectral function of $A$, having the following eight properties:*

1. *$E(\varnothing) = 0$ and $E(\mathbb{R}) = \mathbf{1}$.*
2. *$E(\Delta) = E(\Delta)^{[*]}$, for all $\Delta \in \mathcal{R}_A$.*
3. *$E(\Delta)E(\Delta') = E(\Delta \cap \Delta')$, for all $\Delta, \Delta' \in \mathcal{R}_A$.*
4. *$E(\Delta) + E(\Delta') = E(\Delta \cup \Delta')$, for all disjoint $\Delta, \Delta' \in \mathcal{R}_A$.*
5. *For any sequence $\{\Delta_n\}_{n\in\mathbb{N}} \subseteq \mathcal{R}_A$ with $\Delta_n \subseteq \Delta_{n+1}$, for all $n \in \mathbb{N}$, and*

$$\Delta := \bigcup_{n\in\mathbb{N}} \Delta_n \ \in \ \mathcal{R}_A \ , \tag{A.41}$$

   *we have, for all $x \in \mathcal{K}$,*

$$E(\Delta_n)x \ \xrightarrow{n\to\infty} \ E(\Delta)x \ . \tag{A.42}$$

6. *For all $\Delta \in \mathcal{R}_A$ such that a definitizing polynomial $p$ is positive (negative) on $\overline{\Delta} \cap \sigma(A)$, the subspace $E(\Delta)\mathcal{K}$ is positive (negative).*

[1] Nothing changes, if we allow for complex polynomials, see [22], p. 11.

7. *$E(\Delta)$ is in the double commutant of $A$, for all $\Delta \in \mathcal{R}_A$.*

8. *$\sigma(A\restriction_{E(\Delta)\mathcal{K}}) \subseteq \overline{\Delta}$, for all $\Delta \in \mathcal{R}_A$.*

*This mapping $E$ is uniquely determined by the properties (1), (3)-(5), (7) and (8).*

Let us remark with regard to property (6) in the above theorem: By Theorem A.5 the subspace $E(\Delta)\mathcal{K}$ is a positive Krein space, for any $\Delta$ such that a definitizing polynomial $p$ is positive on $\overline{\Delta} \cap \sigma(A)$. As we have previously remarked, it is therefore an Hilbert space with the scalar product $[\cdot\,|\,\cdot]\restriction_{E(\Delta)\mathcal{K}}$.

We prove the uniqueness assertion in Theorem A.7.

**Lemma A.8.** *For any Banach space $X$ and $A \in \mathcal{B}(X)$, let $\tilde{\mathcal{R}}$ be the semi-ring generated by all intervals in $\mathbb{R}$ with endpoints not in some finite set $c \in \mathbb{R}$ and the complements of these intervals in $\mathbb{R}$. Suppose*

$$E : \tilde{\mathcal{R}} \to \mathcal{B}(X) \tag{A.43}$$

*is an operator-valued function satisfying all properties of Theorem A.7, except (2) and (6). Then $E$ is unique.*

*Proof:* Let $A \in \mathcal{B}(X)$ and $\tilde{\mathcal{R}}$ be the semi-ring specified above. Assume we are given two operator-valued functions $E_1$ and $E_2$

$$E_\iota : \tilde{\mathcal{R}} \longrightarrow \mathcal{B}(X) \quad , \qquad \forall\, \iota \in \{1,2\} \tag{A.44}$$

fulfilling the hypothesis of the lemma. First of all, it is easy to see that

$$[E_\iota(\Delta), A] = \mathbf{0} \quad , \qquad \forall\, \Delta \in \tilde{\mathcal{R}},\ \iota \in \{1,2\}\ , \tag{A.45}$$

since $A$ is of course an element of its own commutant and since $E_1$ and $E_2$ both satisfy property (7). Therefore, we may even conclude

$$[E_1(\Delta_1), E_2(\Delta_2)] = \mathbf{0} \quad , \qquad \forall\, \Delta_1, \Delta_2 \in \tilde{\mathcal{R}}\ , \tag{A.46}$$

since, again due to the fact that $E_2$ satisfies property (7), we have

$$[E_1(\Delta_1), A] = \mathbf{0} \quad \Rightarrow \quad [E_1(\Delta_1), E_2(\Delta_2)] = \mathbf{0}\ , \tag{A.47}$$

for all $\Delta_1, \Delta_2 \in \tilde{\mathcal{R}}$. We show next that, for any $\Delta_1, \Delta_2 \in \tilde{\mathcal{R}}$, we have

$$\sigma := \sigma\left(A\restriction_{E_1(\Delta_1)E_2(\Delta_2)\mathcal{K}}\right) \ \subseteq\ \overline{\Delta}_1 \cap \overline{\Delta}_2\ . \tag{A.48}$$

We first show that

$$\sigma \subseteq \mathbb{R}\ . \tag{A.49}$$

Assume we had $\lambda_0 \in \sigma \cap (\mathbb{C} \setminus \mathbb{R})$. Since $A\restriction_{E_1(\Delta)E_2(\Delta)\mathcal{K}}$ is bounded, we may additionally assume that $\lambda_0$ is not an interior point of $\sigma$. The existence of a sequence $\{x_n\}_{n\in\mathbb{N}}$ in $E_1(\Delta_1)E_2(\Delta_2)\mathcal{K}$ with

$$\|\, x_n \,\| = 1\ , \quad \forall\, n \in \mathbb{N}\ , \qquad \text{and} \qquad \|\, (A - \lambda \cdot \mathbf{1})x_n \,\| \ \xrightarrow{n\to\infty}\ 0 \tag{A.50}$$

follows. Since, however, (A.46) implies $\{x_n\}_{n\in\mathbb{N}} \subseteq E_1(\Delta_1)\mathcal{K}$, we have

$$\lambda_0 \in \sigma\left(A\restriction_{E_1(\Delta)\mathcal{K}}\right) \ , \tag{A.51}$$

in contradiction to property (8). We have thus shown (A.49).

Similarly, assume we had $\lambda \in \sigma \setminus \overline{\Delta}_1$. Due to (A.49), $\lambda$ is not an interior point of $\sigma$ (seen as a subset of $\mathbb{C}$). This again entails the existence of a sequence $\{x_n\}_{n\in\mathbb{N}}$ in $E_1(\Delta_1)E_2(\Delta_2)\mathcal{K}$, such that

$$\|\, x_n \,\| = 1 \ , \quad \forall\, n \in \mathbb{N} \ , \qquad \text{and} \qquad \|\, (A - \lambda \cdot \mathbf{1})x_n \,\| \ \xrightarrow{n\to\infty} \ 0 \ . \tag{A.52}$$

Again by (A.46) it follows that $x_n \in E_1(\Delta_1)\mathcal{K}$, for all $n \in \mathbb{N}$, and thus

$$\lambda \in \sigma\left(A\restriction_{E_1(\Delta_1)\mathcal{K}}\right) \subseteq \overline{\Delta}_1 \ , \tag{A.53}$$

in contradiction to our assumption. Since the same argument may be repeated with the roles of $\Delta_1$ and $\Delta_2$ and the roles of $E_1$ and $E_2$ interchanged, we have proved (A.48).

In particular, this shows

$$\operatorname{dist}(\Delta_1, \Delta_2) > 0 \quad \Rightarrow \quad E_1(\Delta_1)E_2(\Delta_2) = \mathbf{0} \quad , \qquad \forall\, \Delta_1, \Delta_2 \in \tilde{\mathcal{R}} \ . \tag{A.54}$$

In order to prove that $E_1$ and $E_2$ coincide, due to properties (4) and (5), it suffices to show that

$$E_1(\Delta) = E_2(\Delta) \ , \tag{A.55}$$

for all open intervals $\Delta \in \tilde{\mathcal{R}}$. Let $\Delta$ be such an open interval in $\tilde{\mathcal{R}}$ and let $\{\Delta_n\}_{n\in\mathbb{N}}$ be a sequence in $\tilde{\mathcal{R}}$ such that

$$\Delta_n \subseteq \Delta_{n+1} \ , \quad \forall\, n \in \mathbb{N} \ , \qquad \text{and} \qquad \Delta = \bigcup_{n\in\mathbb{N}} \Delta_n \ , \tag{A.56}$$

obeying the additional property

$$\operatorname{dist}(\Delta_n, \mathbb{R} \setminus \Delta) > 0 \quad , \qquad \forall\, n \in \mathbb{N} \ . \tag{A.57}$$

Then it follows from (A.54) and by property (5)

$$E_1(\Delta)E_2(\mathbb{R} \setminus \Delta)x = \lim_{n\to\infty} \left(E_1(\Delta_n)E_2(\mathbb{R} \setminus \Delta)x\right) = 0 \quad , \qquad \forall\, x \in \mathcal{K} \ . \tag{A.58}$$

By property (1) this implies

$$E_1(\Delta) - E_1(\Delta)E_2(\Delta) = E_1(\Delta)E_2(\mathbb{R} \setminus \Delta) = \mathbf{0} \ . \tag{A.59}$$

Since the same argument can be repeated with the roles of $E_1$ and $E_2$ interchanged, we obtain by (A.46) and (A.59)

$$E_1(\Delta) = E_1(\Delta)E_2(\Delta) = E_2(\Delta)E_1(\Delta) = E_2(\Delta) \quad , \qquad \forall\, \Delta \in \tilde{\mathcal{R}} \ . \tag{A.60}$$

The lemma is proved. □

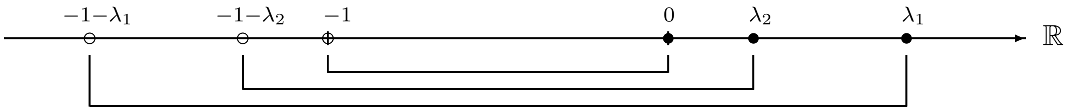


Figure A.1: The eigenvalues belonging to eigenvectors which are not negative are marked with solid disclets. The eigenvalues belonging to eigenvectors which are not positive are marked with blank disclets. Pairs of eigenvalues associated by (A.63) are joined with brackets.

Let us remark that, for a nonnegative $A \in \mathcal{B}(\mathcal{K})$, we have

$$E\big([-\parallel A \parallel, \parallel A \parallel]\big) = \mathbf{1} \qquad \text{and} \qquad E\big(\mathbb{R} \setminus [-\parallel A \parallel, \parallel A \parallel]\big) = \mathbf{0}\ . \tag{A.61}$$

We now consider the case of an admissible, bosonic generalized density matrix $\Gamma \in \mathcal{B}(\mathcal{K})$. Before we turn to the proof of Lemma 3.12, let us first sketch the situation. To this end, we assume that to each $\lambda$ in the spectrum of $\Gamma$ there exists an eigenvector $x$. Then we have by assumed non-negativity of $\Gamma$, for all eigenvalues $\lambda$ with a corresponding eigenvector $x$ in $\mathcal{K}$,

$$\lambda\, [x \,|\, x] = [x \,|\, \Gamma x] \geq 0\ . \tag{A.62}$$

On the other hand, we have by relation (3.38)

$$\Gamma x = \lambda x \qquad \Leftrightarrow \qquad \Gamma(\tau x) = (-1-\lambda)(\tau x) \tag{A.63}$$

and thus we have a situation as we have sketched in Figure A.1. Note, that the conjugation $\tau$ maps positive vectors to negative vectors and vice-versa, leaving the set of neutral vectors invariant.

We now restate and prove Lemma 3.12.

**Lemma A.9.** *To a given generalized density matrix $\Gamma \in \mathcal{B}(\mathcal{K})$, there exists a fundamental decomposition $\mathcal{K} = \tilde{\mathcal{K}}_+ [+] \tilde{\mathcal{K}}_-$ into subspaces*[2]*, invariant under the action of $\Gamma$, with the additional self-duality property $\tau\tilde{\mathcal{K}}_\pm = \tilde{\mathcal{K}}_\mp$. $\Gamma$ has no critical points.*

*Proof:* We first note that by relation (1.58) the operator $-\tau\Gamma\tau$ is nonnegative. Thus it follows from relation (3.38) that, apart from $id$, also $q$ with $q(t) = t + 1$ is a definitizing polynomial for $\Gamma$. Since these two polynomials have no zeros in common, it follows that $\Gamma$ possesses no critical points. By Theorem A.7, the operator $\Gamma$ therefore has a spectral function

$$E : \mathcal{R} \to \mathcal{B}(\mathcal{K})\ , \tag{A.64}$$

where $\mathcal{R}$ denotes the semi-ring generated by all bounded intervals in $\mathbb{R}$ and their complements in $\mathbb{R}$.

[2] The existence of invariant subspaces has been shown even for general nonnegative bounded operators (see Theorem 7.1 in [22]). However, the proof is in our case considerably easier and we additionally show that this is, in the present case, due to the absence of critical points.

Let $\Delta$ be any interval such that $\overline{\Delta} \subseteq (-1,0)$. By the nonnegativity of $\Gamma$ and property (6) of the spectral function, we have that $E(\Delta)\mathcal{K}$ is a negative Krein space. Similarly, we have, by the fact that $q(\Gamma)$ is a nonnegative operator, that $E(\Delta)\mathcal{K}$ is a positive Krein space. It must therefore be trivial, i. e., $E(\Delta) = \mathbf{0}$. Since this is true for all closed intervals contained in $(-1,0)$, it follows by properties (1), (5) and (8) that

$$E\big((-1,0)\big) = \mathbf{0} \qquad \text{or equivalently} \qquad E\big([-\,\|\,\Gamma\,\|\,,\|\,\Gamma\,\|] \setminus (-1,0)\big) = \mathbf{1}\ . \tag{A.65}$$

We now construct a fundamental decomposition of $\mathcal{K}$ into subspaces invariant under the action of $\Gamma$: Any convex combination of definitizing polynomials is again a definitizing polynomial. Hence, apart from $id$ and $q$, also $\tilde{q}$ with $\tilde{q}(t) = t + \frac{1}{2}$ is a definitizing polynomial of $\Gamma$. Thus it follows from property (6) that, with

$$\tilde{\mathcal{K}}_+ := E(\Delta_+)\mathcal{K} \qquad \text{and} \qquad \tilde{\mathcal{K}}_- := E(\Delta_-)\mathcal{K} \tag{A.66}$$

with

$$\Delta_+ := [0, \|\,\Gamma\,\|] \qquad \text{and} \qquad \Delta_- := [-\,\|\,\Gamma\,\|\,, -1]\ , \tag{A.67}$$

$\tilde{\mathcal{K}}_+$ is a positive Krein space and $\tilde{\mathcal{K}}_-$ is a negative Krein space. From (A.65) and property (3) we have that

$$\mathcal{K} = \tilde{\mathcal{K}}_+ {}^{[+]}\, \tilde{\mathcal{K}}_- \tag{A.68}$$

is indeed a fundamental decomposition into invariant subspaces of $\Gamma$.

It just remains to prove self-duality. Let us remark that by Lemma A.8

$$\Delta \in \mathcal{R} \ \mapsto\ E(\Delta)\restriction_{\tilde{\mathcal{K}}_\pm} \tag{A.69}$$

is the spectral function of the operator $\Gamma\restriction_{\tilde{\mathcal{K}}_\pm}$, which is selfadjoint in the Hilbert space $\tilde{\mathcal{K}}_\pm$, see p. 34 in [22]. Furthermore, by property (8), we have

$$\sigma\left(\Gamma\restriction_{\tilde{\mathcal{K}}_\pm}\right) \subseteq \Delta_\pm\ . \tag{A.70}$$

Suppose $\{p_n\}_{n\in\mathbb{N}}$ is a sequence of real polynomials such that

$$p_n(t) \ \xrightarrow{n\to\infty}\ 1 \qquad\qquad \forall\ t \in \Delta_+ \tag{A.71}$$

and

$$p_n(t) \ \xrightarrow{n\to\infty}\ 0 \qquad\qquad \forall\ t \in \Delta_- \tag{A.72}$$

uniformly in $t$. Due to relation (3.38) and the fact that $\tau^2 = \mathbf{1}$, we have

$$\tau p_n(\Gamma)\tau = p_n(-\mathbf{1} - \Gamma) \qquad\qquad \forall\ n \in \mathbb{N}\ . \tag{A.73}$$

We now take the limit of this relation, as $n \to \infty$. Consider any $x \in \mathcal{K}$ and decompose it with respect to (A.68), i. e.,

$$x = \tilde{x}_+ + \tilde{x}_- \qquad \text{such that} \qquad \tilde{x}_\pm \in \tilde{\mathcal{K}}_\pm\ . \tag{A.74}$$

Since $\tilde{\mathcal{K}}_\pm$ are invariant subspaces of $\Gamma$, we have, as $n \to \infty$,

$$p_n(\Gamma)x = p_n\left(\Gamma\restriction_{\tilde{\mathcal{K}}_+}\right)\tilde{x}_+ + p_n\left(\Gamma\restriction_{\tilde{\mathcal{K}}_-}\right)\tilde{x}_- \longrightarrow E(\Delta_+)\tilde{x}_+ = E(\Delta_+)x\ , \tag{A.75}$$

where we have used (A.70) and the functional calculus in the Hilbert spaces $\tilde{\mathcal{K}}_\pm$. Similarly, we have, as $n \to \infty$,

$$p_n(-\mathbf{1} - \Gamma)x = p_n\left((-\mathbf{1} - \Gamma)\restriction_{\tilde{\mathcal{K}}_+}\right)\tilde{x}_+ + p_n\left((-\mathbf{1} - \Gamma)\restriction_{\tilde{\mathcal{K}}_-}\right)\tilde{x}_- \longrightarrow \\ E(\Delta_-)\tilde{x}_- = E(\Delta_-)x \ , \quad \text{(A.76)}$$

since

$$p_n(-1 - t) \xrightarrow{n\to\infty} 0 \qquad \forall\, t \in \Delta_+ \tag{A.77}$$

and

$$p_n(-1 - t) \xrightarrow{n\to\infty} 1 \qquad \forall\, t \in \Delta_- \ , \tag{A.78}$$

uniformly in $t$. The last two statements together with (A.73) yield

$$\tau E(\Delta_+)\tau = E(\Delta_-) \ . \tag{A.79}$$

This proves $\tau\tilde{\mathcal{K}}_\pm = \tilde{\mathcal{K}}_\mp$. $\square$

# Appendix B

# Normal-Ordering

## B.1 Normal-Ordering of Boson Fields

**Definition B.1.** *Let $f \in \mathcal{H}^1$ be given. Then we define, for arbitrary $n \in \mathbb{N}_0$, the* *normal-ordered monomials* $:\Phi(f)^n:$ *as the unique polynomials in $\Phi(f)$ of degree $n$ with leading coefficient 1, obeying the property*

$$:\Phi(f)^n:\Omega \;\in\; \mathcal{H}^n_+ \tag{B.1}$$

*and extend this definition by linearity to all polynomials in $\Phi(f)$.*

In other words, the application of the Gram-Schmidt procedure to the family of linearly independent vectors given by $\{\Phi(f)^n\Omega\}_{n\in\mathbb{N}}$ results in the family $\{:\Phi(f)^n:\Omega\}_{n\in\mathbb{N}}$ of orthogonal vectors.

In the Schrödinger representation it is easily seen that this corresponds to orthogonalizing the monomials $\{x^n\}_{n\in\mathbb{N}_0}$ with respect to a Gaussian measure. Therefore, we have

$$:\Phi(f)^n: = 2^{-\frac{n}{2}} H_n\big(\sqrt{2}\Phi(f)\big) \;, \tag{B.2}$$

where $H_n$ denotes the $n$-th Hermite polynomial. For a proof of this fact, we refer the reader to Sections 1.5 and 6.3 in [18]. Furthermore, the following binomial formula holds.

$$:\Phi(f)^n: = 2^{-\frac{n}{2}} \sum_{l=0}^{n} \binom{n}{l} a^*(f)^l a(f)^{n-l} \quad , \qquad \forall\, n \in \mathbb{N}_0 \;. \tag{B.3}$$

Note that we can make sense out of identities (B.2) and (B.3) either on the domain of finite vectors or in the sense of expectation values in analytic states, only. This is, however, sufficient for our purpose.

Let us now define, for arbitrary $f \in \mathcal{H}^1$ and any $\alpha \in \mathbb{C}$, an operator in $\mathcal{F}_+$ by setting

$$e^{\alpha\Phi(f)}\psi := \sum_{n=0}^{\infty} \frac{\alpha^n}{n!}\Phi(f)^n\psi \qquad \text{and} \qquad :e^{\alpha\Phi(f)}:\psi := \sum_{n=0}^{\infty} \frac{\alpha^n}{n!}:\Phi(f)^n:\psi \;, \tag{B.4}$$

for all vectors

$$\psi \in \bigcap_{n=1}^{\infty} \mathcal{D}\big(\Phi(f)^n\big) \tag{B.5}$$

such that the series in (B.4) converge in norm. An estimate similar to (1.40) shows that they converge at least on the subspace of finite vectors. By relation (B.3) we also obtain:

$$:e^{\alpha\Phi(f)}:\psi = e^{\frac{\alpha}{\sqrt{2}}a^*(f)} e^{\frac{\alpha}{\sqrt{2}}a(f)}\psi \quad , \qquad \forall\, \pi \in F_+ \ . \tag{B.6}$$

"Much of the combinatorics of Wick monomials (i. e. normal-ordered monomials) is summarized by" (Glimm and Jaffe in [18, p. 109]):

$$:e^{\alpha\Phi(f)}:\psi = e^{-\frac{\alpha^2}{4}} e^{\alpha\Phi(f)}\psi \quad , \qquad \forall\, f \in \mathcal{H}^1,\ \|\, f\,\| = 1,\ \alpha \in \mathbb{C},\ \psi \in F_+ \ . \tag{B.7}$$

*Proof:* We use the following representation of the Hermite polynomials

$$H_n(x) := \sum_{j=0}^{\lfloor \frac{n}{2} \rfloor} (-1)^j \frac{n!}{(n-2j)!2^j j!} x^{n-2j} \quad , \qquad \forall\, n \in \mathbb{N}_0\ ,\ x \in \mathbb{R}\ . \tag{B.8}$$

We use this relation to calculate the left hand side (l. h. s.) of the claim (B.7). Using (B.2), we have

$$\begin{aligned}
\text{l. h. s.} &= \lim_{K\to\infty} \sum_{k=0}^{K} \alpha^k \sum_{j=0}^{\lfloor \frac{k}{2} \rfloor} \frac{(-1)^j}{(k-2j)!2^{2j} j!} \Phi(f)^{k-2j}\psi \\
&= \lim_{K\to\infty} \sum_{j=0}^{K} \sum_{k=j}^{K} \frac{(-1)^j}{2^{2j} j!} \left\{ \frac{\alpha^{2k}}{(2k-2j)!} \Phi(f)^{2k-2j}\psi + \frac{\alpha^{2k+1}}{(2k+1-2j)} \Phi(f)^{2k+1-2j}\psi \right\} \\
&= \lim_{K\to\infty} \sum_{j=0}^{K} \sum_{k=0}^{K-j} \frac{\left(\frac{-\alpha^2}{4}\right)^j}{j!} \left\{ \frac{\alpha^{2k}}{(2k)!} \Phi(f)^{2k}\psi + \frac{\alpha^{2k+1}}{(2k+1)!} \Phi(f)^{2k+1}\psi \right\} \\
&= \sum_{j=0}^{\infty} \frac{\left(-\frac{\alpha^2}{4}\right)^j}{j!} \sum_{k=0}^{\infty} \frac{\alpha^k}{k!} \Phi(f)^k \psi \\
&= \text{r. h. s.}\ .
\end{aligned} \tag{B.9}$$

In the last step we have decoupled the limit of the two series as in the Cauchy product formula. Namely, it is possible, to change the order of summation according to

$$\lim_{K\to\infty} \sum_{j=0}^{K} \sum_{k=0}^{K-j} a_j b_k = \lim_{K\to\infty} \sum_{l=0}^{K} \sum_{p+q=l} a_p b_q = \left( \sum_{k=0}^{\infty} a_k \right) \left( \sum_{k=0}^{\infty} b_k \right) \ , \tag{B.10}$$

for all sequences $a$ and $b$ such that the series on the right hand side converge. (In the present context, the convergence in norm corresponds to absolute convergence.) □

## B.2 Normal-Ordering of Annihilation and Creation Operators

In this section we extend the notion of normal-ordering to arbitrary polynomials of either boson or fermion annihilation and creation operators. This step is not completely unproblematic, because we must from now on distinguish between polynomials in the annihilation and creation operators and the algebra element represented by these polynomials. For instance, for any $f_1, f_2, f_3 \in \mathcal{H}^1$, the polynomial expressions

$$a(f_1)a^*(f_2)a(f_3) \qquad \text{and} \qquad \langle f_1 \,|\, f_2 \rangle\, a(f_3) + a^*(f_2)a(f_1)a(f_3) \tag{B.11}$$

in the boson case and

$$a(f_1)a^*(f_2)a(f_3) \qquad \text{and} \qquad \langle f_1 \,|\, f_2 \rangle\, a(f_3) - a^*(f_2)a(f_1)a(f_3) \tag{B.12}$$

in the fermion case are different as polynomials. Nonetheless they do represent the same algebra element[1], due to the CCR and CAR, respectively. The normal-ordering we are now about to introduce is defined on the polynomial expressions in the annihilation and creation operators. It will turn out that it is *not* well-defined on the corresponding algebra.

**Definition B.2.** *Let $\varepsilon = 1$ in the boson case and $\varepsilon = -1$ in the fermion case. Denote by $a(\cdot)$ and $a^*(\cdot)$ the generators of the CCR and CAR Algebra, respectively. We then associate to any monomial*

$$a^{\tau_1}(f_1)\cdots a^{\tau_n}(f_n) \quad , \qquad \forall\, n \in \mathbb{N},\ \tau_1, \ldots, \tau_n \in \{\varnothing, *\},\ f_1, \ldots, f_n \in \mathcal{H}^1 \ , \tag{B.13}$$

*a monomial, normal-ordered with respect to the Fock representation, by defining*

$$:a^{\tau_1}(f_1)\cdots a^{\tau_n}(f_n): \ := \ \varepsilon^{\pi} \cdot a^{\tau_{\pi(1)}}(f_{\pi(1)}) \cdots a^{\tau_{\pi(n)}}(f_{\pi(n)}) \ . \tag{B.14}$$

*The permutation $\pi$ is uniquely determined by the conditions*

$$\tau_{\pi(1)} = \cdots = \tau_{\pi(k)} = * \quad , \quad \tau_{\pi(k+1)} = \cdots = \tau_{\pi(n)} = \varnothing \ , \tag{B.15}$$

*for some $k \in \{0, \ldots, n\}$, and*

$$\pi(1) < \cdots < \pi(k) \quad , \quad \pi(k+1) < \cdots < \pi(n) \ . \tag{B.16}$$

*By demanding linearity and setting $:\mathbf{1}: := \mathbf{1}$, we extend this definition to all polynomials in the boson/fermion annihilation and creation operators and the identity.*

Returning to our previous examples, we have in the boson case

$$:a(f_1)a^*(f_2)a(f_3): \ = \ a^*(f_2)a(f_1)a(f_3) \ , \tag{B.17}$$

but

$$:\big(\langle f_1 \,|\, f_2 \rangle\, a(f_3) + a^*(f_2)a(f_1)a(f_3)\big): \ = \ \langle f_1 \,|\, f_2 \rangle\, a(f_3) + a^*(f_2)a(f_1)a(f_3) \tag{B.18}$$

[1] In the boson case, we can state equality only on the domain of finite vectors

and in the fermion case

$$:a(f_1)a^*(f_2)a(f_3): \;=\; -a^*(f_2)a(f_1)a(f_3)\;, \tag{B.19}$$

but

$$:\big(\langle f_1\,|\,f_2\rangle\,a(f_3) - a^*(f_2)a(f_1)a(f_3)\big): \;=\; \langle f_1\,|\,f_2\rangle\,a(f_3) - a^*(f_2)a(f_1)a(f_3)\;. \tag{B.20}$$

From this example it is clear that the normal-ordering is *not* well-defined on the corresponding algebra

We now define the normal-ordering with respect to another representation of the CCR Algebra and the CAR Algebra, respectively. We consider such representations obtained from the Fock representation by a Bogoliubov transformation.

**Definition B.3.** *Let a bosonic or, respectively, fermionic Bogoliubov transformation $(w,v)$ be given. We define the* <u>*normal-ordering with respect to $(w,v)$*</u> *by the following:*

$$:B(f_1)\cdots B(f_n):_{(w,v)} \;:=\; \alpha^{-1}_{(w,v)}\Big(:\alpha_{(w,v)}\big(B(f_1)\cdots B(f_n)\big):\Big)\;, \tag{B.21}$$

*for all vectors $f_1,\ldots,f_n$ in $\mathcal{K}$ or $\mathcal{L}$, respectively. We denoted by $\alpha_{(w,v)}$ the algebra automorphism associated to $(w,v)$.*

# Appendix C

# The Grassmann Algebra

## C.1 The Grassmann Algebra

**Definition C.1.** *For any Hilbert space $\mathcal{G}$, consider the Hilbert space $\mathcal{G}_2$ given by column vectors with two entries from $\mathcal{G}$, i. e.,*

$$\mathcal{G}_2 := \left\{ \begin{pmatrix} f_1 \\ f_2 \end{pmatrix} \;\middle|\; f_1, f_2 \in \mathcal{G} \right\} \ . \tag{C.1}$$

*We introduce the following (anti-)linear functionals with values in $\mathcal{A}_{car}(\mathcal{G}_2)$:*

$$\xi(f) := a\left( \begin{pmatrix} f \\ 0 \end{pmatrix} \right) \qquad and \qquad \xi^*(f) := a^*\left( \begin{pmatrix} 0 \\ f \end{pmatrix} \right) \quad , \qquad \forall\, f \in \mathcal{G} \ . \tag{C.2}$$

*The norm closure of all polynomials*

$$p\big(\xi^{\sigma_1}(f_1), \ldots, \xi^{\sigma_n}(f_n)\big) \quad , \qquad \forall\, \sigma_1, \ldots, \sigma_n \in \{\varnothing, *\},\ f_1, \ldots, f_n \in \mathcal{G} \ , \tag{C.3}$$

*is called the Grassmann Algebra and is denoted by $\mathcal{A}_{grass}(\mathcal{G})$. Viewing the correspondence given by $\xi(f) \mapsto \xi^*(f)$ as an anti-linear conjugation mapping in the Grassmann Algebra, turns it into a $C^*$-algebra. For any orthonormal set $f_1, \ldots, f_k \in \mathcal{G}$, the algebra elements $\xi(f_1), \xi^*(f_1), \ldots, \xi(f_k), \xi^*(f_k)$ are called Grassmann variables*[1]*.*

Note that the Grassmann Algebra over $\mathcal{G}$ is indeed smaller than the CAR Algebra $\mathcal{A}_{car}(\mathcal{G}_2)$.

The Grassmann variables are introduced in such a way that any variable anti-commutes with any other variable. Note that this implies that only a finite number of linearly independent polynomials can be constructed from any finite set of Grassmann variables, since $\xi(f)^2 = 0$ and $\xi^*(f)^2 = 0$, for any $f \in \mathcal{G}$. This fact allows us to introduce a simple functional calculus on the polynomials in Grassmann variables. Let $g$ be a function of one complex variable, given by a power-series

$$g(x) = \sum_{k=0}^{\infty} a_k x^k \tag{C.4}$$

[1] The traditional term 'variable' is probably motivated by the introduction of the Grassmann integral, see (C.7). However, we would like to emphasize that it is misleading, because $\xi(f)$ and $\xi^*(f)$ are 'fixed' operators and by no means 'variable'.

convergent in some neighborhood of zero. We may then define, for any polynomial expression $p$ involving only a finite number of Grassmann variables,

$$g(p) := \sum_{k=0}^{\infty} a_k \, p^k \ . \tag{C.5}$$

Note that all but finitely many terms in this series actually vanish. Hence, we need not address the question of convergence.

Let us now introduce a linear mapping on all polynomials in finitely many Grassmann variables by the following definitions: Given a complete orthonormal set $\{f_k\}_{k\in K}$ of vectors in $\mathcal{G}$, with $K = \{1, \dots, L\}$ and $L \in \mathbb{N} \cup \{\infty\}$, we define[2], for any $m \in K$:

$$\begin{aligned} \xi^{\sigma_1}(f_1)\cdots\xi^{\sigma_m}(f_m) \ &\mapsto \ \int \xi^{\sigma_1}(f_1)\cdots\xi^{\sigma_m}(f_m)\, d\xi^{\sigma}(f) \\ &:= \sum_{l=1}^{m} (-1)^{m-l} \delta_{\sigma,\sigma_l} \left\langle f^{\sigma} \mid f_l^{\sigma_l} \right\rangle \xi^{\sigma_1}(f_1)\cdots\widehat{\xi^{\sigma_l}(f_l)}\cdots\xi^{\sigma_m}(f_m) \ , \end{aligned} \tag{C.7}$$

for all $\sigma, \sigma_1, \dots, \sigma_m \in \{\varnothing, *\}$ and all $f \in \mathcal{G}$. We use $f^*$ to denote $\bar{f}$ and $f^{\varnothing}$ to denote just $f$. Of particular importance is the case, when $f = f_{k_0}$ is itself a member of the orthonormal set $\{f_k\}_{k\in K}$. In this case, we have

$$\begin{aligned} &\int \xi^{\sigma_1}(f_1)\cdots\xi^{\sigma_m}(f_m)\, d\xi^{\sigma}(f_{k_0}) \\ &\qquad = \begin{cases} (-1)^{m-k_0}\xi^{\sigma_1}(f_1)\cdots\widehat{\xi^{\sigma_{k_0}}(f_{k_0})}\cdots\xi^{\sigma_m}(f_m) & k_0 \in \{1,\dots,m\} \wedge \sigma = \sigma_{k_0} \\ 0 & k_0 \notin \{1,\dots,m\} \vee \sigma \neq \sigma_{k_0} \end{cases} \ , \end{aligned} \tag{C.8}$$

for all $\sigma, \sigma_1, \dots, \sigma_m \in \{\varnothing, *\}$

Compositions of such mappings are written as 'iterated integrals' in the obvious manner. Any such integral is called Grassmann integral. However, we would like to emphasize that, in spite of some formal analogies, it is by no means a true integral. For example, exchanging the order of integration of any two subsequent Grassmann integrations over one variable each, results in a change of sign. We write down the following rule of thumb:

$$d\xi^{\sigma_{\pi(1)}}(f_{\pi(1)})\cdots d\xi^{\sigma_{\pi(m)}}(f_{\pi(m)}) \ = \ \mathrm{sign}(\pi)\cdot d\xi^{\sigma_1}(f_1)\cdots d\xi^{\sigma_m}(f_m) \ , \tag{C.9}$$

for all permutations $\pi \in S_m$.

**Lemma C.2.** *Let $f_k, f_1, \dots, f_m$ be elements of an orthonormal set of vectors in $\mathcal{G}$, not necessarily all distinct from each other, and let $\sigma, \sigma_k, \sigma_1, \dots, \sigma_m \in \{\varnothing, *\}$ be arbitrary. For any polynomial $p$ in $m$ non-commuting variables, we have*

$$\begin{aligned} &\int p\big(\xi^{\sigma_1}(f_1),\dots,\xi^{\sigma_m}(f_m)\big)\big(\xi^{\sigma_k}(f_k) - \xi^{\sigma}(f)\big)d\xi^{\sigma_k}(f_k) \\ &\qquad = p\big(\xi^{\sigma_1}(f_1),\dots,\xi^{\sigma_{k-1}}(f_{k-1}),\xi^{\sigma}(f),\xi^{\sigma_{k+1}}(f_{k+1}),\dots,\xi^{\sigma_m}(f_m)\big) \ , \end{aligned} \tag{C.10}$$

*for any $f \in \mathcal{G}$, where $f$ must be orthogonal to $f_k$ or $\sigma$ distinct from $\sigma_k$.*

[2] The careful reader might observe that the Grassmann integral is in fact an anti-commutator. Namely:

$$\int \xi^{\sigma_1}(f_1)\cdots\xi^{\sigma_m}(f_m)\, d\xi^{\sigma}(f) = \{\xi^{\sigma_1}(f_1)\cdots\xi^{\sigma_m}(f_m), \xi^{\sigma}(f)\} \tag{C.6}$$

*Proof:* By linearity it suffices to prove the lemma under the additional assumption that

$$p\big(\xi^{\sigma_1}(f_1),\ldots,\xi^{\sigma_m}(f_m)\big) = \xi^{\sigma_1}(f_1)\cdots\xi^{\sigma_m}(f_m)\ . \tag{C.11}$$

In this case we have:

$$\begin{aligned}\int \xi^{\sigma_1}(f_1)\cdots\xi^{\sigma_m}(f_m)\big(\xi^{\sigma_k}(f_k)-\xi^{\sigma}(f)\big)\, d\xi^{\sigma_k}(f_k)& \\ = \sum_{l=1}^{m}(-1)^{m+1-l}\,\langle f_l\,|\,f_k\rangle \xi^{\sigma_1}(f_1)\cdots\widehat{\xi^{\sigma_k}(f_l)}\cdots\xi^{\sigma_m}(f_m)\big(\xi^{\sigma_k}(f_k)-\xi^{\sigma}(f)\big)& \\ +\xi^{\sigma_1}(f_1)\cdots\xi^{\sigma_m}(f_m)\ .&\end{aligned} \tag{C.12}$$

The term involving the summation on the right hand side evaluates to zero if none of the $f_1,\ldots,f_m$ is equal to $f_k$; otherwise it evaluates to

$$-\xi^{\sigma_1}(f_1)\cdots\xi^{\sigma_m}(f_m) \ +\ \xi^{\sigma_1}(f_1)\cdots\xi^{\sigma_{k-1}}(f_{k-1})\xi^{\sigma}(f)\xi^{\sigma_{k+1}}(f_{k+1})\cdots\xi^{\sigma_m}(f_m)\ . \tag{C.13}$$

This relation together with (C.12) proves the lemma. □

We now establish a link between the Grassmann Algebra and the many-fermion system defined over the one-particle space $\mathcal{H}^1$. For this purpose, consider the case when $\mathcal{G}$ is given by $n$ orthogonal copies of $\mathcal{H}^1$, such that

$$\mathcal{G} = \underbrace{\mathcal{H}^1\oplus\cdots\oplus\mathcal{H}^1}_{n \text{ entries}}\ . \tag{C.14}$$

We denote the Grassmann variables associated to each of the copies of $\mathcal{H}^1$ by the different symbols $\xi_1,\ldots,\xi_n$, i. e.,

$$\xi_1(f) := \xi(f\oplus 0\oplus\cdots\oplus 0)\ ,\ \ldots\ ,\ \xi_n(f) := \xi(0\oplus\cdots\oplus 0\oplus f) \tag{C.15}$$

and

$$\xi_1^*(f) := \xi^*(f\oplus 0\oplus\cdots\oplus 0)\ ,\ \ldots\ ,\ \xi_n^*(f) := \xi^*(0\oplus\cdots\oplus 0\oplus f)\ , \tag{C.16}$$

for all $f\in\mathcal{H}^1$. Given an orthonormal system $\{f_k\}_{k\in K}$ in $\mathcal{H}^1$, we say, for any $j\in\{1,\ldots,n\}$, that the functional $\xi_j$ corresponds to one set of Grassmann variables given by $\{\xi_j(f_k),\xi_j^*(f_k)\}_{k\in K}$.

Let us now fix an orthonormal basis $\{f_k\}_{k\in\mathbb{N}}$ in $\mathcal{H}^1$ and introduce some notation with respect to this basis. For a given positive integer $\kappa$ and any $j\in\{1,\ldots,n\}$, we define the 'row vectors' of Grassmann variables associated to the first $\kappa$ elements of the basis:

$$(\xi_j)_\kappa := \big(\xi_j(f_1),\ldots,\xi_j(f_\kappa)\big) \qquad \text{and} \qquad (\xi_j^*)_\kappa := \big(\xi_j^*(f_1),\ldots,\xi_j^*(f_\kappa)\big)\ . \tag{C.17}$$

Furthermore, we define the following bilinear form

$$(\xi_j^{\sigma})_\kappa\cdot(\xi_{j'}^{\sigma'})_\kappa := \sum_{k=1}^{\kappa}\xi_j^{\sigma}(f_k)\xi_{j'}^{\sigma'}(f_k)\ , \tag{C.18}$$

for any $j, j' \in \{1, \ldots, n\}$ and arbitrary $\sigma, \sigma' \in \{\varnothing, *\}$. To any multi-index $\underline{s} \in \{0,1\}^\kappa$ we associate the following monomials

$$(\xi_j)^{\underline{s}}_\kappa := \big(\xi_j(f_\kappa)\big)^{s_\kappa} \cdots \big(\xi_j(f_1)\big)^{s_1} , \tag{C.19}$$

$$(\xi^*_j)^{\underline{s}}_\kappa := \big(\xi^*_j(f_1)\big)^{s_1} \cdots \big(\xi^*_j(f_\kappa)\big)^{s_\kappa} , \tag{C.20}$$

where factors of the type $(\cdot)^0$ are understood to be absent. With the help of the notation we just introduced, we may write down the following relations:

$$\exp\big((\xi^*_j)_\kappa \cdot (\xi_{j'})_\kappa\big) = \sum_{\underline{s}\in\{0,1\}^\kappa} (\xi^*_j)^{\underline{s}}_\kappa (\xi_{j'})^{\underline{s}}_\kappa \quad , \qquad \forall\, j, j' \in \{1, \ldots, n\} , \tag{C.21a}$$

and correspondingly

$$\exp\big((\xi_j)_\kappa \cdot (\xi^*_{j'})_\kappa\big) = \sum_{\underline{s}\in\{0,1\}^\kappa} (\xi_j)^{\underline{s}}_\kappa (\xi^*_{j'})^{\underline{s}}_\kappa \quad , \qquad \forall\, j, j' \in \{1, \ldots, n\} . \tag{C.21b}$$

The proof of these relations is immediate. As far as Grassmann integrals are concerned, the most important cases are given by integrals over all the variables $\xi_j(f_1), \ldots, \xi_j(f_\kappa)$ or all the variables $\xi^*_j(f_1), \ldots, \xi^*_j(f_\kappa)$, for a given $j \in \{1, \ldots, n\}$ and any positive integer $\kappa$. We denote these integrals according to the following scheme:

$$\int \cdots (d\xi_j)_\kappa := \int \cdots d\xi_j(f_1) \cdots d\xi_j(f_\kappa) , \tag{C.22}$$

$$\int \cdots (d\xi^*_j)_\kappa := \int \cdots d\xi^*_j(f_\kappa) \cdots d\xi^*_j(f_1) . \tag{C.23}$$

Note the different order of integration. Such integrals can be characterized by

$$\int (\xi^\sigma_j)^{\underline{s}}_\kappa \, (d\xi^\sigma_j)_\kappa = \begin{cases} 1 & \text{if } s_1 = \cdots = s_\kappa = 1 \\ 0 & \text{else} \end{cases} \quad , \quad \forall\, \sigma \in \{\varnothing, *\},\ j \in \{1, \ldots, n\} , \tag{C.24}$$

for all multi-indices $\underline{s} \in \{0,1\}^\kappa$. Based on the previous lemma and relations (C.21), we now prove the main combinatorial result concerning Grassmann variables.

**Lemma C.3.** *Let a positive integer $\kappa$ be given and $j_0 \in \{1, \ldots, n\}$ be arbitrary. Then: For any polynomial expression $p$ in the Grassmann variables*

$$\big\{\xi^\sigma_j(f_k) \mid \sigma \in \{\varnothing, *\},\ j \in \{1, \ldots, n\},\ k \in \{1, \ldots, \kappa\}\big\} \setminus \big\{\xi^*_{j_0}(f_1), \ldots, \xi^*_{j_0}(f_\kappa)\big\} , \tag{C.25}$$

*we have*

$$\int p \, \exp\big((\xi_l - \xi_{l'})_\kappa \cdot (\xi^*_{j_0})_\kappa\big) \, (d\xi^*_{j_0})_\kappa (d\xi_l)_\kappa = p\,|_{\xi_l \to \xi_{l'}} , \tag{C.26}$$

*for any different $l, l' \in \{1, \ldots, n\}$.*

*For any polynomial expression $p$ in the Grassmann variables*

$$\big\{\xi^\sigma_j(f_k) \mid \sigma \in \{\varnothing, *\},\ j \in \{1, \ldots, n\},\ k \in \{1, \ldots, \kappa\}\big\} \setminus \{\xi_{j_0}(f_1), \ldots, \xi_{j_0}(f_\kappa)\} , \tag{C.27}$$

*we have*

$$\int p \, \exp\big((\xi^*_l - \xi^*_{l'})_\kappa \cdot (\xi_{j_0})_\kappa\big) \, (d\xi_{j_0})_\kappa (d\xi^*_l)_\kappa = p\,|_{\xi^*_l \to \xi^*_{l'}} , \tag{C.28}$$

*for any different $l, l' \in \{1, \ldots, n\}$.*

*The notation on the right hand sides of* (C.26) *and* (C.28) *indicates that any* $\xi_l^\sigma(f_k)$ *appearing in the expression* $p$ *is to be replaced by* $\xi_{l'}^\sigma(f_k)$*, for all* $k \in \{1, \ldots, \kappa\}$ *and for* $\sigma = \varnothing$ *or* $\sigma = *$*, respectively.*

*Proof:* We shall only prove (C.26), the proof of (C.28) being completely analogous. By hypothesis, $p$ does not contain any variable of the type $\xi_{j0}^*(f_k)$ and so we can carry out the inner integration on the left hand side of the claim, using relation (C.21b):

$$\int \exp\left((\xi_l - \xi_{l'})_\kappa \cdot (\xi_{j0}^*)_\kappa\right) \, (d\xi_{j0}^*)_\kappa = \sum_{\underline{s} \in \{0,1\}^\kappa} (\xi_l - \xi_{l'})_\kappa^{\underline{s}} \int (\xi_{j0}^*)^{\underline{s}} \, (d\xi_{j0}^*)_\kappa \overset{(C.24)}{=}$$

$$= (\xi_l - \xi_{l'})_\kappa \int (\xi_{j0}^*) \, (d\xi_{j0}^*)_\kappa = (\xi_l - \xi_{l'})_\kappa \; . \tag{C.29}$$

Here, we denote

$$(\xi_l - \xi_{l'})_\kappa := \big(\xi_l(f_1) - \xi_{l'}(f_1), \ldots, \xi_l(f_\kappa) - \xi_{l'}(f_\kappa)\big) \; . \tag{C.30}$$

Thus the left hand side of the claim is equal to

$$\int p \cdot (\xi_l - \xi_{l'})_\kappa \, (d\xi_l)_\kappa$$

$$= \int p \cdot \big(\xi_l(f_\kappa) - \xi_{l'}(f_\kappa)\big) \cdots \big(\xi_l(f_1) - \xi_{l'}(f_1)\big) \, d\xi_l(f_1) \cdots d\xi_l(f_\kappa) \; . \tag{C.31}$$

Applying Lemma C.2 $\kappa$-times completes the proof. □

## C.2 Bounds on Grassmann Gaussian Integrals

For the purpose of our considerations in Subsection 3.2.4, we now introduce a family of norms on algebras generated by finitely many Grassmann variables. We follow the presentation in Appendix B in [30]. Let $\mathcal{G}$ be a Hilbert space and $f_1, \ldots, f_\kappa \in \mathcal{G}$, pairwise orthogonal, be given. Furthermore, denote by $\xi(\cdot)$ the generator of the Grassmann Algebra $\mathcal{A}_{grass}(\mathcal{G})$. Any polynomial expression $p$ in the Grassmann variables $\xi(f_1), \xi^*(f_1), \ldots, \xi(f_\kappa), \xi^*(f_\kappa)$ can be brought into the form

$$p = \sum_{\underline{r}, \underline{s} \in \{0,1\}^\kappa} \alpha_{\underline{r}, \underline{s}} \, (\xi^*)_\kappa^{\underline{r}} (\xi)_\kappa^{\underline{s}} \quad , \tag{C.32}$$

for some complex numbers $\{\alpha_{\underline{r},\underline{s}}\}_{\underline{r},\underline{s} \in \{0,1\}^\kappa}$. We may then define, for any fixed $q > 0$, the norm $\| \cdot \|_q$, by setting:

$$\| p \|_q := \sum_{\underline{r}, \underline{s} \in \{0,1\}^\kappa} | \alpha_{\underline{r},\underline{s}} | \, q^{\frac{1}{2}(|\underline{r}| + |\underline{s}|)} \; , \tag{C.33}$$

where, for any multi-index $\underline{m} \in \{0, 1\}^\kappa$, we set

$$| \underline{m} | := \sum_{k=1}^{\kappa} m_k \; . \tag{C.34}$$

The linear independence of the monomials $\{(\xi^*)^{\underline{r}}_{k}, (\xi)^{\underline{s}}_{k}\}_{\underline{r},\underline{s}\in\{0,1\}^\kappa}$ guarantees that the above defines in fact a norm. Furthermore, we have the following inequality

$$\| \, p\,\tilde{p} \, \|_q \leq \| \, p \, \|_q \, \| \, \tilde{p} \, \|_q \ , \tag{C.35}$$

for any two polynomial expressions $p$ and $\tilde{p}$.

*Proof of* (C.35)*:* Let $p$ and $\tilde{p}$ be of the form

$$p = \sum_{\underline{r},\underline{s}\in\{0,1\}^\kappa} \alpha_{\underline{r},\underline{s}} \, (\xi^*)^{\underline{r}}_{\kappa} (\xi)^{\underline{s}}_{\kappa} \qquad \text{and} \qquad \tilde{p} = \sum_{\underline{\tilde{r}},\underline{\tilde{s}}\in\{0,1\}^\kappa} \tilde{\alpha}_{\underline{\tilde{r}},\underline{\tilde{s}}} \, (\xi^*)^{\underline{\tilde{r}}}_{\kappa} (\xi)^{\underline{\tilde{s}}}_{\kappa} \ . \tag{C.36}$$

We then have

$$\begin{aligned} \| \, p\,\tilde{p} \, \|_q &\leq \sum_{\underline{r},\underline{s},\underline{\tilde{r}},\underline{\tilde{s}}\in\{0,1\}^\kappa} | \, \alpha_{\underline{r},\underline{s}} \, | \, | \, \tilde{\alpha}_{\underline{\tilde{r}},\underline{\tilde{s}}} \, | \, \| \, (\xi^*)^{\underline{r}}_{\kappa} (\xi)^{\underline{s}}_{\kappa} (\xi^*)^{\underline{\tilde{r}}}_{\kappa} (\xi)^{\underline{\tilde{s}}}_{\kappa} \, \|_q \\ &\leq \sum_{\underline{r},\underline{s},\underline{\tilde{r}},\underline{\tilde{s}}\in\{0,1\}^\kappa} | \, \alpha_{\underline{r},\underline{s}} \, | \, | \, \tilde{\alpha}_{\underline{\tilde{r}},\underline{\tilde{s}}} \, | \, q^{\frac{1}{2}(|\,\underline{r}\,|+|\,\underline{s}\,|+|\,\underline{\tilde{r}}\,|+|\,\underline{\tilde{s}}\,|)} = \| \, p \, \|_q \, \| \, \tilde{p} \, \|_q \ , \end{aligned} \tag{C.37}$$

where we have first used the triangle inequality and then estimated the norm of the monomials, some of which are actually zero. □

Let us point out that if $\mathcal{G}$ is given by (C.14), we have thus defined a norm on the finite polynomial expressions in all the $n$ sets of Grassmann variables.

We now quote the main theorem of this section from [30]:

**Theorem C.4.** *Let $C$ be an invertible $\kappa \times \kappa$ matrix allowing a representation of the type*

$$C_{i,j} = \langle a_i \, | \, b_j \, \rangle_{\mathcal{V}} \ , \tag{C.38}$$

*where $a_1, \ldots, a_\kappa$ and $b_1, \ldots, b_\kappa$ are elements of some separable Hilbert space $\mathcal{V}$ and $\| \, a_i \, \|_{\mathcal{V}} \leq q$ and $\| \, b_i \, \|_{\mathcal{V}} \leq q$, for all $i \in \{1, \ldots, \kappa\}$ and some some $q > 0$ independent of $i$. We then have*

$$\left| \det C \int \exp\left[ \sum_{i,i'=1}^{\kappa} \xi^*(f_i)(C^{-1})_{i,i'} \xi(f_{i'}) \right] p\big((\xi^*)_\kappa; (\xi)_\kappa\big) \right| \leq \| \, p\big((\xi^*)_\kappa; (\xi)_\kappa\big) \, \|_q \ , \tag{C.39}$$

*for any polynomial $p$.*

We remind the reader that in this section we would like to show that we can reexponentiate in (3.259) according to (3.262). In order to prove this, we consider the following error integral:

$$\begin{aligned} E_N(\beta) := \int \exp\left[ \sum_{l,l'=1}^{N} Q_{l,l'} \, (\xi^*_l)_\kappa \cdot (\xi_{l'})_\kappa \right] \exp\Big[ (\xi_N)_\kappa \cdot (\eta^*)_\kappa + (\eta)_\kappa \cdot (\xi^*_1)_\kappa \Big] \\ \left\{ \prod_{j=1}^{N} e^{-\frac{\beta}{N} H_\kappa(\xi^*_j, \xi_j)} - \prod_{j=1}^{N} \left( \mathbf{1} - \frac{\beta}{N} H_\kappa(\xi^*_j, \xi_j) \right) \right\} \prod_{j=1}^{N} (d\xi_j)_\kappa (d\xi^*_j)_\kappa \ . \end{aligned} \tag{C.40}$$

Let us start with the following two observations: First, we have quite trivially

$$\exp\big((\xi_N)_\kappa \cdot (\eta^*)_\kappa + (\eta)_\kappa \cdot (\xi_1^*)_\kappa\big) \;=\; \sum_{\underline{r},\underline{s}\in\{0,1\}^\kappa} (-1)^{|\,\underline{r}\,|^2} (\eta^*)_\kappa^{\underline{r}} (\eta)_\kappa^{\underline{s}} (\xi_1^*)_\kappa^{\underline{s}} (\xi_N)_\kappa^{\underline{r}} \tag{C.41}$$

by relations (C.21). Secondly, on denoting the expressions in the curly braces of (C.40) by $R_N(\beta)$, we observe

$$\begin{aligned} R_N(\beta) &= \sum_{\substack{S\dot\cup T=\{1,\dots,N\}\\ T\neq\emptyset}} \prod_{s\in S}\left(1-\frac{\beta}{N}H_\kappa(\xi_s^*,\xi_s)\right)\prod_{t\in T}\left(\sum_{r=2}^\infty \frac{1}{r!}\left(-\frac{\beta}{N}H_\kappa(\xi_t^*,\xi_t)\right)^r\right) \\ &= \sum_{\substack{S\dot\cup T=\{1,\dots,N\}\\ T\neq\emptyset}} \sum_{U\subseteq S}\prod_{u\in U}\left(-\frac{\beta}{N}H_\kappa(\xi_u^*,\xi_u)\right) \sum_{\underline{r}\in\{2,3,\dots\}^T}\prod_{t\in T}\left(\frac{1}{r_t!}\left(-\frac{\beta}{N}H_\kappa(\xi_t^*,\xi_t)\right)^{r_t}\right). \end{aligned} \tag{C.42}$$

By the properties of the Grassmann variables, this expression is in fact a polynomial in $\beta$, and it is easy to read off that all its monomials are of degree two or higher. Therefore, we may write

$$R_N(\beta) = \sum_{p=2}^\infty \beta^p R_{N,p} \tag{C.43}$$

with

$$R_{N,p} \;:=\; \sum{}' \prod_{u\in U}\left(-\frac{1}{N}H_\kappa(\xi_u^*,\xi_u)\right)\prod_{t\in T}\left(\frac{1}{r_t!}\left(-\frac{1}{N}H_\kappa(\xi_t^*,\xi_t)\right)^{r_t}\right)\;, \tag{C.44}$$

where the summation $\sum'$ extends over all $S\dot\cup T$ with $T\neq\emptyset$, all $U\subseteq S$ and all $\underline{r}\in\{2,3,\dots\}^T$, such that $|\,U\,|+\sum_{t\in T} r_t = p$. Combining (C.41) with this last observation, we see that we may express $E_N(\beta)$ in the following way

$$E_N(\beta) = \sum_{p=2}^\infty \beta^p E_{N,p}\;, \tag{C.45}$$

where the Grassmann quantities $E_{N,p}$ are given by

$$E_{N,p} = \sum_{\underline{r},\underline{s}\in\{0,1\}^\kappa} (-1)^{|\,\underline{r}\,|^2} (\eta^*)_\kappa^{\underline{r}} (\eta)_\kappa^{\underline{s}} E_{N,p}^{\underline{r},\underline{s}} \tag{C.46}$$

and finally, the complex numbers $E_{N,p}^{\underline{r},\underline{s}}$ are given in terms of the following Grassmann integral:

$$E_{N,p}^{\underline{r},\underline{s}} = \int \exp\left[\sum_{l,l'=1}^N Q_{l,l'}\,(\xi_l^*)_\kappa\cdot(\xi_{l'})_\kappa\right] (\xi_1^*)_\kappa^{\underline{r}}(\xi_N)_\kappa^{\underline{s}}\, R_{N,p} \prod_{j=1}^N (d\xi_j)_\kappa (d\xi_j^*)_\kappa\;. \tag{C.47}$$

In order to achieve our goal of proving that we may reexponentiate in (3.259), we shall show that

$$E_{N,p}\longrightarrow 0 \qquad \text{as} \qquad N\longrightarrow\infty\;, \tag{C.48}$$

for all $p$ in any norm on the Grassmann Algebra generated by $\eta(f_1), \eta^*(f_1), \ldots, \eta(f_\kappa), \eta^*(f_\kappa)$. (Remember that this is a finite dimensional vector space and hence, all its norms are equivalent.) Since the sum in (C.46) is finite, it suffices to show that

$$E^{\underline{r},\underline{s}}_{N,p} \longrightarrow 0 \qquad \text{as} \qquad N \longrightarrow \infty \; , \tag{C.49}$$

for all multi-indices $\underline{r}, \underline{s} \in \{0,1\}^\kappa$ and all $p \in \{2,3,\ldots\}$. This will be achieved with the aid of Theorem C.4. In order to make this machinery work, we need to do two things:

(i) We need to show that the covariance given by $Q$ in (3.260) satisfies the hypothesis of this theorem, for a suitable $q > 0$.

(ii) We need to derive some bounds on the integrand in (C.47) with respect to the norm $\|\cdot\|_q$.

Part (i) is accomplished by the following lemma.

**Lemma C.5.** *Define the Matrix $C$ as the inverse of $Q$, which is in turn defined by* (3.260)*. On labeling the entries of $C$ by two pairs of indices, the first index in each pair labeling the block and the second index in each pair corresponding to the entries within each block, we have the following representation of $C$:*

$$C_{m_1,k_1;m_2,k_2} = \langle a_{m_1,k_1} \,|\, b_{m_2,k_2} \rangle \qquad \forall\, m_1, m_2 \in \{1,\ldots,N\} \; , \quad \forall\, k_1, k_2 \in \{1,\ldots,\kappa\} \; , \tag{C.50}$$

*the vectors $a_{m_1,k_1}$ and $b_{m_2,k_2}$ being given by:*

$$a_{m_1,k_1} \;:=\; \frac{1}{\sqrt{N}} \begin{pmatrix} \frac{1}{\sqrt{|1-\mathcal{Z}_1|}} \mathcal{Z}_1^{N-m_1} \\ \vdots \\ \frac{1}{\sqrt{|1-\mathcal{Z}_N|}} \mathcal{Z}_N^{N-m_1} \end{pmatrix} \otimes e^{k_1} \; , \tag{C.51}$$

$$b_{m_2,k_2} \;:=\; \frac{1}{\sqrt{N}} \begin{pmatrix} \frac{\sqrt{|1-\mathcal{Z}_1|}}{1-\mathcal{Z}_1} \mathcal{Z}_1^{N-m_2} \\ \vdots \\ \frac{\sqrt{|1-\mathcal{Z}_N|}}{1-\mathcal{Z}_N} \mathcal{Z}_N^{N-m_2} \end{pmatrix} \otimes e^{k_2} \; . \tag{C.52}$$

*Here, we have denoted by*

$$\mathcal{Z}_m \;:=\; \exp\left(i\frac{\pi}{N}(2m-1)\right) \quad , \qquad \forall\, m \in \{1,\ldots,N\} \; , \tag{C.53}$$

*the $N$-th roots of $-1$ and by $\mathrm{e}^1, \ldots, e^\kappa$ the standard basis in the linear space of column vectors with $\kappa$ complex entries. Furthermore, we have*

$$\|\, a_{m_1,k_1} \|^2 = \|\, b_{m_2,k_2} \|^2 \leq \frac{1}{2^{3/2}} \left(3 + \ln\left(\frac{N}{2}\right)\right) \; . \tag{C.54}$$

*Proof:* First we prove the representation (C.50). Note that $Q$ may be written in the form of a tensor product of an $N \times N$ matrix and the $\kappa \times \kappa$ unity matrix in the following way:

$$\tilde{Q} := JQJ^{-1} = \begin{pmatrix} 1 & & & 1 \\ -1 & \ddots & & \\ & \ddots & \ddots & \\ & & -1 & 1 \end{pmatrix} \otimes \mathbf{1}_\kappa \ , \tag{C.55}$$

with respect to the unitary mapping $J : \mathbb{C}^{N\cdot\kappa} \to \mathbb{C}^N \otimes \mathbb{C}^\kappa$, which is given by

$$J \begin{pmatrix} x_1 \\ \vdots \\ x_N \end{pmatrix} := \sum_{m=1}^{N} e^m \otimes x_m \quad , \qquad \forall\ x_1, \ldots, x_N \in \mathbb{C}^\kappa \ . \tag{C.56}$$

The eigenvalue problem for $\tilde{Q}$ is solved by

$$\tilde{Q} X_{m,k} = (1 - \mathcal{Z}_m) \cdot X_{k,m} \quad , \qquad \forall\ m \in \{1, \ldots, N\},\ k \in \{1, \ldots, \kappa\} \ , \tag{C.57}$$

where we have denoted by

$$X_{m,k} := \frac{1}{\sqrt{N}} \begin{pmatrix} \mathcal{Z}_m^{N-1} \\ \vdots \\ \mathcal{Z}_m^0 \end{pmatrix} \otimes e^k \ , \quad \text{with} \qquad \mathcal{Z}_m := \exp\left(\frac{i\pi}{N}(2m-1)\right) \ , \tag{C.58}$$

the eigenvectors of $\tilde{Q}$. The family of vectors $\{X_{m,k}\}_{m,k}$ is easily seen to form an orthonormal basis in $\mathbb{C}^N \otimes \mathbb{C}^\kappa$. Viewing $\tilde{C} := \tilde{Q}^{-1}$ as a linear mapping, we therefore have

$$\tilde{C} = \frac{1}{N} \sum_{\substack{k \in \{1,\ldots,\kappa\}\,, \\ m \in \{1,\ldots,N\}}} \frac{1}{1 - \mathcal{Z}_m} \left\langle X_{m,k} \,|\, \cdot \,\right\rangle X_{m,k} \ . \tag{C.59}$$

This leads to the following conclusion concerning the matrix elements of the matrix $C$:

$$\begin{aligned} C_{m_1,k_1;m_2,k_2} &= \left\langle e^{m_1} \otimes e^{k_1} \,\middle|\, \tilde{C} e^{m_2} \otimes e^{k_2} \right\rangle \qquad \text{(C.60)} \\ &= \frac{1}{N} \sum_{\substack{k \in \{1,\ldots,\kappa\} \\ m \in \{1,\ldots,N\}}} \frac{1}{1 - \mathcal{Z}_m} \left\langle e^{m_1} \otimes e^{k_1} \,|\, X_{m,k} \right\rangle \left\langle X_{m,k} \,\middle|\, e^{m_2} \otimes e^{k_2} \right\rangle \\ &= \frac{1}{N} \sum_{\substack{k \in \{1,\ldots,\kappa\} \\ m \in \{1,\ldots,N\}}} \left\{ \left\langle e^{m_1} \otimes e^{k_1} \,|\, X_{m,k} \right\rangle \frac{1}{|\, 1 - \mathcal{Z}_m \,|^{\frac{1}{2}}} \right\} \\ &\qquad\qquad \left\{ \frac{|\, 1 - \mathcal{Z}_m \,|^{\frac{1}{2}}}{1 - \mathcal{Z}_m} \left\langle X_{m_1,k_1} \,\middle|\, e^{m_2} \otimes e^{k_2} \right\rangle \right\} \\ &= \frac{1}{N} \sum_{\substack{k \in \{1,\ldots,\kappa\} \\ m \in \{1,\ldots,N\}}} \left\{ \frac{1}{|\, 1 - \mathcal{Z}_m \,|^{\frac{1}{2}}} \mathcal{Z}_m^{N-m_1} \delta_{k_1,k} \right\} \left\{ \frac{|\, 1 - \mathcal{Z}_m \,|^{\frac{1}{2}}}{1 - \mathcal{Z}_m} \mathcal{Z}_m^{N-m_2} \delta_{k,k_2} \right\} \ , \end{aligned}$$

for all $m_1, m_2 \in \{1, \dots N\}$ and $k_1, k_2 \in \{1, \dots, \kappa\}$. The two curly braces in the above expression correspond to the vectors $a_{m_1,k_1}$ and $b_{m_2,k_2}$, respectively. This completes the first part of the proof.

We now prove the bound (C.54) on the vectors $a_{m_1,k_1}$. To this end, let us assume, without loss of generality, that $N$ is an even number. In this case, the norm squared of $a_{m_1,k_1}$ is given by

$$N \cdot \| a_{m_1,k_1} \|^2 = \sum_{m=-\frac{N}{4}+\frac{1}{2}}^{\frac{3N}{4}-\frac{1}{2}} \frac{1}{|\, 1 - \mathcal{Z}_m \,|} = \sum_{m=-\frac{N}{4}+\frac{1}{2}}^{\frac{N}{4}+\frac{1}{2}} \frac{1}{|\, 1 - \mathcal{Z}_m \,|} + \sum_{m=\frac{N}{4}+\frac{3}{2}}^{\frac{3N}{4}-\frac{1}{2}} \frac{1}{|\, 1 - \mathcal{Z}_m \,|} \; . \tag{C.61}$$

Recall (C.46). In the first of the two sums on the right hand side, the modulus of the argument of $\mathcal{Z}_m$ is always in $[-\frac{\pi}{2}, \frac{\pi}{2}]$, while in the second sum it is always outside of $(-\frac{\pi}{2}, \frac{\pi}{2})$. We now estimate these two sums separately, according to the following inequality

$$\left|\, 1 - e^{i\alpha} \,\right| \geq \sqrt{2} \cdot \begin{cases} \frac{2}{\pi} \,|\, \alpha \,| & \text{if } |\, \alpha \,| \leq \frac{\pi}{2} \\ 1 & \text{if } |\, \alpha \,| \geq \frac{\pi}{2} \end{cases} \quad , \qquad \forall\, \alpha \in [-\pi, \pi] \; . \tag{C.62}$$

This yields, for the first of the two sums,

$$\begin{aligned} \sum_{m=-\frac{N}{4}+\frac{1}{2}}^{\frac{N}{4}+\frac{1}{2}} \frac{1}{|\, 1 - \mathcal{Z}_m \,|} &\leq \frac{N}{2^{\frac{3}{2}}} \sum_{m=-\frac{N}{4}+\frac{1}{2}}^{\frac{N}{4}+\frac{1}{2}} \frac{1}{|\, 2m - 1 \,|} \\ &= \frac{N}{2^{\frac{3}{2}}} \left( \sum_{m=-\frac{N}{4}+\frac{1}{2}}^{-1} \frac{1}{|\, 1 - \mathcal{Z}_m \,|} + 2 + \sum_{m=2}^{\frac{N}{4}+\frac{1}{2}} \frac{1}{|\, 1 - \mathcal{Z}_m \,|} \right) \\ &\leq \frac{N}{2^{\frac{3}{2}}} \left( \frac{1}{2} \ln\left(\frac{N}{2}\right) + 2 + \frac{1}{2} \ln\left(\frac{N}{2}\right) \right) \quad , \end{aligned} \tag{C.63}$$

while the second sum is simply estimated by

$$\sum_{m=\frac{N}{4}+\frac{3}{2}}^{\frac{3N}{4}-\frac{1}{2}} \frac{1}{|\, 1 - \mathcal{Z}_m \,|} \leq \sum_{m=\frac{N}{4}+\frac{3}{2}}^{\frac{3N}{4}-\frac{1}{2}} \frac{1}{\sqrt{2}} = \frac{1}{\sqrt{2}} \left( \frac{N}{2} - 1 \right) \leq \frac{N}{2^{\frac{3}{2}}} \; . \tag{C.64}$$

On reinserting these estimates in (C.61), we readily obtain:

$$\| a_{m,k} \|^2 \leq \frac{1}{2^{\frac{3}{2}}} \left( \ln\left(\frac{N}{2}\right) + 3 \right) - \frac{1}{\sqrt{2}} \; . \tag{C.65}$$

The estimate of $\| b_{m_2,k_2} \|^2$ is completely analogous. $\square$

The following norm estimate on one of the factors in the integrand of (C.47) is an important step to accomplishing part (ii).

**Theorem C.6.** *There exist constants $c, d > 0$ such that*

$$\| R_{N,p} \|_q \leq c\, q^{2\kappa p} N^{-d} \tag{C.66}$$

*holds true, for all $q > 1$ and sufficiently large $N$.*

*Proof:* Since any polynomial expression in $2\kappa$ Grassmann variables is of degree $2\kappa$ or lower, there exist nonnegative numbers $a_1, a_2, \ldots$ such that

$$\| H_\kappa(\xi^*, \xi)^r \|_q \leq a_r\, q^{2\kappa} \ , \tag{C.67}$$

for all $q \geq 1$ and all positive integers $r$. In fact, all but finitely many of these numbers can be chosen to be zero, since any polynomial in $\{\xi_j(f_k), \xi_j^*(f_k)\}_{j\in\{1,\ldots,n\},\ k\in\{1,\ldots,\kappa\}}$ is nilpotent. Let us suppose, the $a_1, a_2, \ldots$ have been chosen in such a way, and set $a := a_1$ and $b := \sum_{r=2}^{\infty} \frac{1}{r!} a_r$. We may then estimate $R_{N,p}$, given in (C.44), according to:

$$\begin{aligned}
\| R_{N,p} \|_q &\leq {\sum}' \prod_{u\in U} \| \tfrac{1}{N} H_\kappa(\xi_u^*, \xi_u) \|_q \prod_{t\in T} \Big\| \tfrac{1}{r_t!} \left(\tfrac{1}{N} H_\kappa(\xi_t^*, \xi_t)\right)^{r_t} \Big\|_q \\
&\leq q^{2\kappa p} \sum_{\substack{S\dot\cup T=\{1,\ldots,N\} \\ T\neq\emptyset}} \sum_{U\subseteq S} \left(\tfrac{1}{N} a\right)^{|U|} \left(\tfrac{1}{N^2} b q^{2\kappa}\right)^{|T|} \\
&\leq q^{2\kappa p} \sum_{\substack{S\dot\cup T=\{1,\ldots,N\} \\ T\neq\emptyset}} \left(1 + \tfrac{1}{N} a\right)^{|S|} \left(\tfrac{1}{N^2} b q^{2\kappa}\right)^{|T|} \\
&= q^{2\kappa p} \left( \left(1 + \tfrac{1}{N} a + \tfrac{1}{N^2} b q^{2\kappa}\right)^N - \left(1 + \tfrac{1}{N} a\right)^N \right) \ ,
\end{aligned}$$

where the summation $\sum'$ is defined as above (see p. 163). We may rewrite the last line to obtain

$$\| R_{N,p} \|_q \leq q^{2\kappa p} \left(1 + \tfrac{1}{N} a\right)^N \left( (1 + x_N)^N - 1 \right) \ , \quad \text{with} \quad x_N := \left(1 - \tfrac{1}{N} a\right)^{-1} \tfrac{1}{N^2} b q^{2\kappa} \ . \tag{C.68}$$

It is now easily observed that

$$(1 + x_N)^N - 1 \leq N x_N e^{N x_N} \qquad \text{and} \qquad N x_N \leq c_0 \cdot N^{-d} \ , \tag{C.69}$$

for some positive constants $c_0$ and $d$. Thus we obtain

$$\| R_{N,p} \|_q \leq q^{2\kappa p} \left(1 + \tfrac{1}{N} a\right)^N c_0 N^{-d} e^{c_0 N^{-d}} \ . \tag{C.70}$$

Since $(1 + \frac{1}{N} a)^N$ and $e^{c_0 N^{-d}}$ converge, as $N \to \infty$, the claim follows. $\square$

We now combine Lemma C.5 and Theorems C.4 and C.6 to build up our argument. The lemma shows that the covariance given by $Q$ satisfies the hypothesis of Theorem C.4, for any $N \in \mathbb{N}$, if we chose the following $q = q_N$:

$$q_N := \frac{1}{2^{\frac{3}{2}}} \left( \ln\left(\frac{N}{2}\right) + 3 \right) \quad , \qquad \forall\, N \in \mathbb{N} \ . \tag{C.71}$$

Thus we obtain, with the help of Theorems C.4 and C.6,

$$\begin{aligned}
\left| E_{N,p}^{\underline{r},\underline{s}} \right| &\leq \det Q \, \| (\xi_1^*)_\kappa^{\underline{r}} (\xi_N)_\kappa^{\underline{s}} \|_{q_N} \| R_{N,p} \|_{q_N} \\
&\leq 2 c q_N^{|\underline{r}|+|\underline{s}|+2\kappa p} N^{-d} \leq 2 c q_N 2\kappa(p+1) N^{-d} \ ,
\end{aligned} \tag{C.72}$$

for sufficiently large $N$ and all $p, \underline{r}, \underline{s}$. We have used $\det Q = 2^\kappa$ and $|\,\underline{r}\,|, |\,\underline{s}\,| \leq \kappa$. Taking into account the behavior of $q_N$ for large $N$, we see that the right hand side tends to zero as $N \to \infty$, for all $p \in \mathbb{N}$. As we have already mentioned, by (C.46) this suffices to show that

$$E_{N,p} \longrightarrow 0 \qquad \text{as} \qquad N \longrightarrow \infty \ . \tag{C.73}$$

We now conclude our argument with the following observations: Denoting the integral in (3.259) by $I_N(\beta)$, after introducing a $\beta$ in the obvious places, we have

$$(3.259) = \lim_{N\to\infty} \big(I_N(\beta)\big)|_{\beta=1} \ . \tag{C.74}$$

We would like to prove that

$$(3.259) = \lim_{N\to\infty} \left(\tilde{I}_N(\beta)\right)|_{\beta=1} \ , \tag{C.75}$$

where we denote by $\tilde{I}_N(\beta)$ the reexponentiated integral, given by

$$\tilde{I}_N(\beta) = \int \exp\left[\big((\xi_1^*)_\kappa, \ldots, (\xi_N^*)_\kappa\big) Q \begin{pmatrix} (\xi_1)_\kappa^T \\ \vdots \\ (\xi_N)_\kappa^T \end{pmatrix}\right] \exp\big((\xi_N)_\kappa \cdot (\eta^*)_\kappa + (\eta)_\kappa \cdot (\xi_1^*)_\kappa\big)$$
$$\exp\left(\sum_{j=1}^N \frac{\beta}{N} H_\kappa(\xi_j^*, \xi_j)\right) \prod_{j=1}^N (d\xi_j)_\kappa (d\xi_j^*)_\kappa \ . \tag{C.76}$$

In order to show this, we remark that both $I_N(\beta)$ and $\tilde{I}_N(\beta)$ are polynomials in $\beta$ of degree at most $N \cdot \kappa$. Hence, we may write

$$I_N(\beta) = \sum_{p=0}^\infty \beta^p I_{N,p} \qquad \text{and} \qquad \tilde{I}_N(\beta) = \sum_{p=0}^\infty \beta^p \tilde{I}_{N,p} \ , \tag{C.77}$$

for suitable Grassmann quantities $I_{N,p}$ and $\tilde{I}_{N,p}$. Therefore, we may conclude

$$\lim_{N\to\infty} I_N(\beta) = \lim_{N\to\infty} \left(\sum_{p=0}^\infty \beta^p I_{N,p}\right) = \lim_{N\to\infty} \left(\sum_{p=0}^\infty \beta^p \left(\tilde{I}_{N,p} - E_{N,p}\right)\right) \ . \tag{C.78}$$

Let us now remind the reader that (3.259) was originally given by

$$\sum_{\underline{m},\underline{n} \in \{0,1\}^\kappa} (\eta)_\kappa^{\underline{m}} (\eta^*)_\kappa^{\underline{n}} \operatorname{tr}\left((a)_\kappa^{\underline{n}} (a)_\kappa^{\underline{m}} P_\kappa e^{-\beta H} P_\kappa\right) \ , \tag{C.79}$$

except for the $\beta$ we have introduced. Now, since we have assumed that $H$ leaves the range of $P_\kappa$ invariant, we may write $P_\kappa e^{-\beta H} P_\kappa$ as $e^{-P_\kappa H P_\kappa}$. Therefore and because the above trace is actually finite dimensional, (3.259) is analytic in $\beta$. This is the essential ingredient to conclude that, since the limit is equal to (3.259) and is analytic, we may in (C.78) interchange the summation over $p$ and the limit $N \to \infty$, by the Cauchy formulae. Thus we have:

$$\lim_{N\to\infty} I_N(\beta) = \lim_{N\to\infty} \tilde{I}_N(\beta) \ , \tag{C.80}$$

by (C.73). This completes our argument.

## C.3 The Grassmann Extension of the CAR Algebra

The peculiarity of the Grassmann extension of the CAR Algebra we are about to introduce is that fermion particle annihilation operators $a(\cdot)$ and fermion particle creation operators $a^*(\cdot)$ appear together with Grassmann variables $\xi^*(\cdot)$ and $\xi(\cdot)$ in one algebra as anti-commuting elements. We then have

$$[a(f)\xi^*(f), \xi(g)a^*(g)] = \langle f \mid g \rangle \, \xi^*(f)\xi(g) \tag{C.81a}$$

and

$$[a(f)\xi^*(f), a(g)\xi^*(g)] = [\xi(f)a^*(f), \xi(g)a^*(g)] = 0 \ , \tag{C.81b}$$

for all $f, g \in \mathcal{H}^1$. The fact that the CAR are thus coded in commutation relations, can simplify some calculations a lot on the combinatorial score.

In order to perform the extension of the CAR Algebra $\mathcal{A}_{\mathrm{car}}(\mathcal{H}^1)$ by one set of Grassmann variables $\mathcal{A}_{\mathrm{grass}}(\mathcal{H}^1)$, we first consider the algebra $\mathcal{A} := \mathcal{A}_{\mathrm{car}}(\mathcal{G}_2 \oplus \mathcal{H}^1)$, where $\mathcal{G}_2 := \mathcal{H}^1 \oplus \mathcal{H}^1$ and the symbol $\oplus$ denotes the orthogonal direct sum of two Hilbert spaces. Evidently, $\mathcal{A}$ contains as sub-algebras

$$\mathcal{A}_{\mathrm{grass}}(\mathcal{H}^1) \subseteq \mathcal{A}_{\mathrm{car}}(\mathcal{G}_2) \subseteq \mathcal{A} \qquad \text{and} \qquad \mathcal{A}_{\mathrm{car}}(\mathcal{H}^1) \subseteq \mathcal{A} \ . \tag{C.82}$$

Note that the $*$-operations are defined differently on the sub-algebras $\mathcal{A}_{\mathrm{grass}}(\mathcal{H}^1)$ and $\mathcal{A}_{\mathrm{car}}(\mathcal{H}^1)$. However, since both are continuous, the norm closure of all polynomials

$$p\big(a^{\sigma_1}(f_1), \ldots, a^{\sigma_m}(f_m); \xi^{\mu_1}(g_1), \ldots, \xi^{\mu_n}(g_n)\big) \ , \tag{C.83}$$

for all $f$'s and $g$'s in $\mathcal{H}^1$ and all $\sigma$s and $\mu$s in $\{\varnothing, *\}$, seen as elements in $\mathcal{A}_{\mathrm{car}}(\mathcal{G}_2 \oplus \mathcal{H}^1)$ is a $C^*$-algebra, which we shall denote by $\hat{\mathcal{A}}_{\mathrm{car}}(\mathcal{H}^1)$. This algebra obviously contains all fermion particle annihilation and creations operators $a(\cdot)$ and respectively $a^*(\cdot)$, as much as all Grassmann variables $\xi^*(\cdot)$ and $\xi(\cdot)$. Any Grassmann variable anti-commutes with any annihilation and any creation operator. We have thus achieved our goal.

Finally, let us remark that it is by no means compulsory to extend the CAR Algebra by precisely the Grassmann Algebra over the same one particle space. In fact, any other Hilbert space can be chosen and the same construction still works. In the commutation relations (C.81) it is equally by no means necessary to pair $a^\sharp(f)$ with $\xi^\sharp(f)$; in fact any Grassmann variable may be used.

# Appendix D

# Some Complementary Lemmas

In this appendix we shall prove some lemmas, which are included in this work for the reader's convenience. Most of them can be found in the literature in one form or the other.

**Lemma D.1.** *If $A$ is a selfadjoint operator and $\psi$ is a corresponding analytic vector, then we have*

$$\psi \in \mathcal{D}\left(e^{itA}\right) \qquad \text{and} \qquad e^{itA}\psi = \lim_{N\to\infty} \sum_{n=0}^{N} \frac{(it)^n A^n}{n!}\psi \tag{D.1}$$

*for any $t \in \mathbb{R}$ with $|\,t\,|$ sufficiently small.*

*Proof:* For any $R > 0$ we shall denote by $P_R$ the projection onto the spectral subspace of $A$ corresponding to $\sigma(A) \cap [-R, R]$. Then the Operator $AP_R$ is bounded for any $R > 0$ and we have

$$e^{itA}P_R\psi = \lim_{N\to\infty}\left(\sum_{n=0}^{N}\frac{(it)^n}{n!}A^n P_R\psi\right) = P_R \lim_{N\to\infty}\left(\sum_{n=0}^{N}\frac{(it)^n}{n!}A^n\psi\right) \tag{D.2}$$

Since we have assumed that $\psi$ is an analytic vector of $A$, the limit $N \to \infty$ on the very right hand side exists and so these expressions have a limit as $R \to \infty$, too. However, $e^{tA}$ is selfadjoint and therefore closed, implying

$$e^{itA}\lim_{R\to\infty} P_R\psi = \lim_{R\to\infty} e^{itA}P_R\psi = \lim_{N\to\infty}\left(\sum_{n=0}^{N}\frac{(it)^n}{n!}A^n\psi\right) \tag{D.3}$$

and thus proving the lemma. □

**Lemma D.2.** *Let $H$ be an operator in $\mathcal{F}_+$ of the form $H = \mathrm{d}\mathbf{G}(c) + B(g)$ for some bounded one-particle operator $c = c^*$ and some $g \in \mathcal{K}_{\mathbb{R}}$. Then*

$$H^k B(f)\psi = \sum_{l=0}^{k}\binom{k}{l}B(C^l f)H^{k-l} + \sum_{l=1}^{k}\binom{k}{l}\left[\tau g \,\middle|\, C^{l-1}f\right]H^{k-l} \tag{D.4}$$

*holds for all $k \in \mathbb{N}$ on the domain $F_+$ of finite vectors, with*

$$C = \begin{pmatrix} c & \mathbf{0} \\ \mathbf{0} & -\bar{c} \end{pmatrix} \tag{D.5}$$

.

*Proof:* All the operator identities in this proof, are to be understood on the domain $F_+$ of finite vectors. We shall prove the lemma by an induction argument with respect to $k$. For $k = 1$ the claim reads:

$$HB(f) = B(f)H + B(Cf) + [\tau g \,|\, f] \tag{D.6}$$

This relation can easily be verified with the help of the CCR, remembering that the strictly quadratic part of $H$ may we written in the from $\sum_{k,k'} \langle f_k \,|\, c f_{k'} \rangle \, a^*(f_k) a(f_{k'})$ for some arbitrary one-particle basis $\{f_k\}_{k \in K_+}$. Now assume the claim was true for one particular $k \in \mathbb{N}$. It then follows:

$$H^{k+1}B(f) = \underbrace{H\left(\sum_{l=0}^{k} \binom{k}{l} B(C^l f) H^{k-l}\right)}_{\text{expression 1}} + \underbrace{H\left(\sum_{l=1}^{k} \binom{k}{l} \left[\tau g \,\middle|\, C^{l-1} f\right] H^{k-l}\right)}_{\text{expression 2}} \tag{D.7}$$

As far as expression 1 is concerned, we have due to (D.6)

$$\begin{aligned}
\text{expression 1} &= \sum_{l=0}^{k} \binom{k}{l} \left(B(C^l f) H^{k+1-l} + B(C^{l+1} f) H^{k-l} + \left[\tau g \,\middle|\, C^l f\right] H^{k-l}\right) \\
&= \sum_{l=0}^{k} \binom{k}{l} B(C^l f) H^{k+1-l} + \sum_{l=1}^{k+1} \binom{k}{l-1} B(C^l f) H^{k+1-l} \\
&+ \sum_{l=1}^{k+1} \binom{k}{l-1} \left[\tau g \,\middle|\, C^{l-1} f\right] H^{k+1-l} \\
&= \sum_{l=0}^{k+1} \binom{k+1}{l} B(C^l f) H^{k+1-l} + \sum_{l=1}^{k+1} \binom{k}{l-1} \left[\tau g \,\middle|\, C^{l-1} f\right] H^{k+1-l} \,.
\end{aligned}$$

As far as expression 2 is concerned, we have

$$\begin{aligned}
\text{expression 2} &= \sum_{l=1}^{k} \binom{k}{l} \left[\tau g \,\middle|\, C^{l-1} f\right] H^{k+1-l} \\
&= \sum_{l=1}^{k+1} \binom{k+1}{l} \left[\tau g \,\middle|\, C^{l-1} f\right] H^{k+1-l} - \sum_{l=1}^{k+1} \binom{k}{l-1} \left[\tau g \,\middle|\, C^{l-1} f\right] H^{k+1-l} \,.
\end{aligned}$$

Inserting the last two formulae into (D.7), we arrive at the identity claimed. □

**Lemma D.3.** *Let $H$ be a selfadjoint operator in $\mathcal{F}_-$ of the form $H = \mathrm{d}\mathbf{G}(c)$ for some one-particle operator $c = c^*$, not necessarily bounded. Then for any $k \in \mathbb{N}$, we have*

$$H^k B(f)\psi = \sum_{l=0}^{k} \binom{k}{l} B(C^l f) H^{k-l} \psi \tag{D.8}$$

*for all $\psi \in F_- \cap \mathcal{D}(\mathrm{d}\mathbf{G}(c))$ and all $f \in \mathcal{D}(C)$, with*

$$C = \begin{pmatrix} c & \mathbf{0} \\ \mathbf{0} & -\bar{c} \end{pmatrix} \,. \tag{D.9}$$

*Proof:* Note that $B(f)\psi$ is also in $F_- \cap \mathcal{D}(\mathrm{d}\mathbf{G}(f)$ It is straightforward to see that

$$\mathrm{d}\mathbf{G}(c)B(f)\psi = B(f)\,\mathrm{d}\mathbf{G}(c)\psi + B(Cf)\psi \tag{D.10}$$

by using the CAR. From now on this proof is exactly the same as the proof of Lemma D.2.

$\square$

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